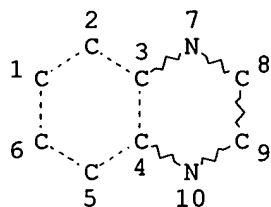


10/088814

(FILE 'REGISTRY' ENTERED AT 09:51:58 ON 07 FEB 2005)

L1 STR

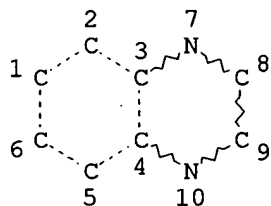


Claim 27

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L3 52883 SEA FILE=REGISTRY SSS FUL L1
L18 STR



NODE ATTRIBUTES:
CONNECT IS X2 RC AT 7
CONNECT IS X2 RC AT 10
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L19 37274 SEA FILE=REGISTRY SUB=L3 SSS FUL L18

100.0% PROCESSED 52883 ITERATIONS
SEARCH TIME: 00.00.01

37274 ANSWERS

(FILE 'CAPLUS' ENTERED AT 09:53:15 ON 07 FEB 2005)

L20 13830 S L19
L21 3262 S L20(L) (RACT OR RCT)/RL
L22 39 S L21(L) PHARM?/RL

L22 ANSWER 1 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 13 Jan 2005
ACCESSION NUMBER: 2005:29314 CAPLUS
TITLE: Preparation of heterocyclic 2-trifluoromethylpentan-2-

Searcher : Shears 571-272-2528

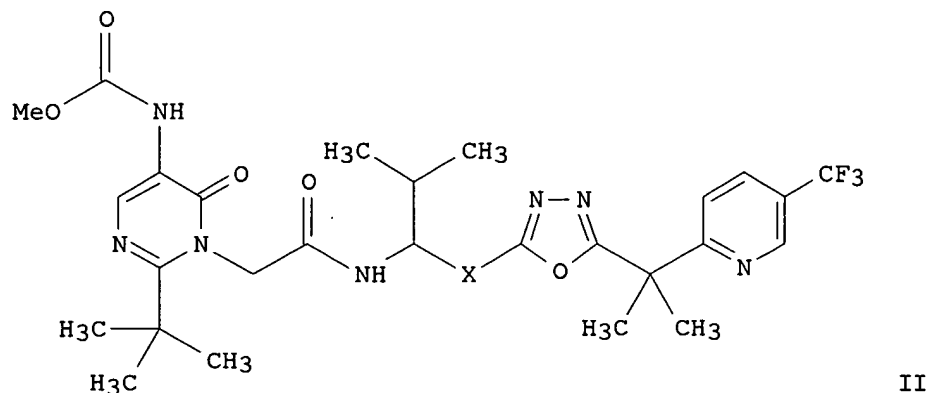
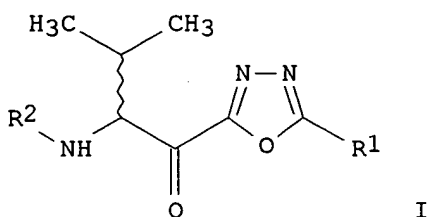
INVENTOR(S): ols and related compounds as anti-inflammatory agents
 Berger, Markus; Baeurle, Stefan; Rehwinkel, Hartmut;
 Schmees, Norbert; Schaecke, Heike; Lehmann, Manfred;
 Krolikiewicz, Konrad; Schottelius, Arndt J. B.;
 Nguyen, Duy; Mengel, Anne; Jaroch, Stefan
 PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
 SOURCE: PCT Int. Appl., 118 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005003098	A1	20050113	WO 2004-EP6765	20040622
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10330358	A1	20050203	DE 2003-10330358	20030701
PRIORITY APPLN. INFO.: DE 2003-10330358 A 20030701 DE 2003-10346939 A 20031006				
AB Title compds. I [A = aryl, benzyl, phenylethyl, etc.; R1, R2 = H, Me, Et, etc.; R3 = (un)substituted alkoxy, alkyl, alkenyl, etc.; B = Me, Et, (un)substituted methylene, etc.; Q = (un)substituted quinazoline, quinoxaline, indazole, etc.] and their pharmaceutically acceptable salts were prepared For example, palladium mediated hydrogenation of imine II, e.g., prepared from 4-(5-fluoro-2-methoxyphenyl)-2-hydroxy-4-methyl-2- trifluoromethylpentanal and 5-amino-2-methylquinazoline, afforded trifluoromethylpentanol III. In a glucocorticoid receptor binding assay, compound III exhibited an IC50 value of 1.8 nM. Compds. I are claimed to be useful as anti-inflammatory agents.				
IT INDEXING IN PROGRESS IT 825653-48-3P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of heterocyclic trifluoromethylpentanols and related compds. as anti-inflammatory agents)				
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT				
L22 ANSWER 2 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN ED Entered STN: 16 Sep 2004 ACCESSION NUMBER: 2004:753404 CAPLUS DOCUMENT NUMBER: 141:277626				

10/088814

TITLE: Preparation of oxadiazole derivatives as elastase inhibitors
 INVENTOR(S): Torisu, Kazuhiko; Kobayashi, Kaoru; Naganawa, Atsushi; Sekioka, Tomohiko; Kawabata, Kazuhito
 PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 207 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004256473	A2	20040916	JP 2003-50563	20030227
PRIORITY APPLN. INFO.:			JP 2003-50563	20030227
OTHER SOURCE(S):	MARPAT 141:277626			
GI				



AB Title compds. I [R1 = monocyclic carbocycle, etc.; R2 = COR12, etc.; R12 = alkyl, etc.] were prepared For example, oxidation of compound II [X = CH(OH)], e.g., prepared from 2-chloro-5-(trifluoromethyl)pyridine in 7 steps, using Dess-Martin reagent gave compound II [X = CO]. In elastase inhibition assays, the IC50 values of compds. I were ≤10 μM. Compds. I are claimed useful for the treatment of chronic articular rheumatism, myocardial infarction, etc. Formulations are given.

IT 757970-18-6P

RL: PAC (Pharmacological activity); RCT (Reactant);
 SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological

Searcher : Shears 571-272-2528

study); PREP (Preparation); **RACT (Reactant or reagent); USES**
(Uses)

(preparation of oxadiazole derivs. as elastase inhibitors for treatment
of chronic articular rheumatism and myocardial infarction)

L22 ANSWER 3 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 08 Jul 2004

ACCESSION NUMBER: 2004:546414 CAPLUS

DOCUMENT NUMBER: 141:89103

TITLE: Preparation of arylquinazolines and related
derivatives for promoting the release of parathyroid
hormone

INVENTOR(S): Altmann, Eva; Beerli, Rene; Gerspacher, Marc; Renaud,
Johanne; Weiler, Sven; Widler, Leo

PATENT ASSIGNEE(S): Novartis Ag, Switz.; Novartis Pharma GmbH

SOURCE: PCT Int. Appl., 190 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056365	A2	20040708	WO 2003-EP14741	20031222
WO 2004056365	A3	20040819		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SY, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				

PRIORITY APPLN. INFO.: GB 2002-30015 A 20021223

OTHER SOURCE(S): MARPAT 141:89103

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [Y = O, S; R1 = OH, SH, halo, NO2, etc.; R2 = halo, alkyl,
alkenyl, etc.; R3 = alkyl, benzyl, etc.] are prepared For instance,
(2-amino-5-((propargyl)oxy)phenyl)(4-isopropylphenyl)methanone is
alkylated with 6-bromomethyl-2,3-dimethoxyquinoxaline (dioxane, K2CO3,
80°, 2 days) and the resulting intermediate treated with sodium
isocyanate to give II. Compds. of the invention have IC50 in the range of
10 nM to 50 µM for the parathyroid calcium-sensing receptor. I are
useful for treating bone conditions associated with increased calcium
depletion or resorption.

IT **717103-60-1P**, [2-[[[(2,3-Dimethoxyquinoxalin-6-yl)methyl]amino]-5-
((prop-2-ynyl)oxy)phenyl](4-isopropylphenyl)methanone

10/088814

RL: PAC (Pharmacological activity); RCT (Reactant);
SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
study); PREP (Preparation); RACT (Reactant or reagent); USES
(Uses)

(arylquinazoline and related derivs. for promoting the release of
parathyroid hormone)

L22 ANSWER 4 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 18 Jun 2004

ACCESSION NUMBER: 2004:493706 CAPLUS

DOCUMENT NUMBER: 141:54330

TITLE: Preparation of novel fused pyrazoles, in particular
pyrrolopyrazoles, as transforming growth factor- β
(TGF- β) signal transduction inhibitors

INVENTOR(S): Beight, Douglas Wade; Burkholder, Timothy Paul;
Decollo, Todd Vincent; Godfrey, Alexander Glenn; Heap,
Charles Raymond; King, Chi-Hsin Richard; Li, Hong-Yu;
McMillen, William Thomas; Sawyer, Jason Scott; Wang,
Yan; Diefenbacher, Clive Gideon; Engler, Thomas
Albert; Malhotra, Sushant; Mundla, Sreenivasa Reedy

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: PCT Int. Appl., 143 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

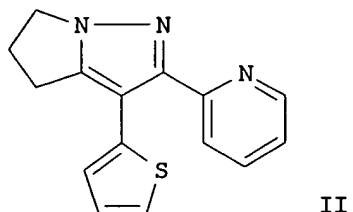
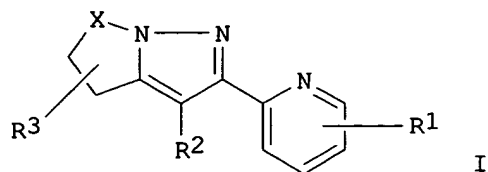
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004050659	A1	20040617	WO 2003-US35969	20031124
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
PRIORITY APPLN. INFO.:			US 2002-429982P	P 20021127
OTHER SOURCE(S):	MARPAT 141:54330			
GI				

Searcher : Shears 571-272-2528

10/088814



AB Title compds. I [wherein X = (CH₂)_n; n = 0-4; R₁ = (un)substituted alk(en/yn)yl, alk(enyl/ynyl)oxy, alkylthio, alkylamino, alkanoyl, alkylcarbamoyl, thiophenyl, Ph, etc.; R₂ = (un)substituted thiophenyl, oxazolyl, pyrazinyl, furanyl, imidazo[1,2-a]pyridinyl, benzoimidazolyl, quinoxalinyl, pyrazolo[1,5-a]pyrimidinyl, [1,8]naphthyridinyl, etc.; R₃ = H, alkyl; and their pharmaceutically acceptable salts] were prepared as transforming growth factor-β (TGF-β) signal transduction inhibitors. II was prepared in 5 steps by Claisen condensation of Et pyridin-2-carboxylate, condensation of β-carbonyl ester with 1-aminopyrrolidin-2-one•HCl, cyclization in the presence of NaOEt in toluene, decarboxylative bromination, and Pd-cross coupling of the bromide with thiophene-2-boronic acid. Selected I inhibited the TGF-β type I receptor kinase domain with IC₅₀ values < 20 μM. I are useful for treating fibroproliferative diseases associated with TGF-β1 over production

IT **705263-39-4P**, 7-[2-(6-Methylpyridin-2-yl)-5,6-dihydro-4H-pyrrolo[1,2-b]pyrazol-3-yl]-1H-quinoxalin-2-one **705263-74-7P**, 2-Chloro-7-[2-(6-methylpyridin-2-yl)-5,6-dihydro-4H-pyrrolo[1,2-b]pyrazol-3-yl]quinoxaline

RL: **PAC (Pharmacological activity); RCT (Reactant);**
SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent); USES**
(Uses)
(TGF-β signal transduction inhibitor; preparation of fused pyrazoles, in particular pyrrolopyrazoles, as TGF-β signal transduction inhibitors)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 5 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 28 May 2004

ACCESSION NUMBER: 2004:433750 CAPLUS

DOCUMENT NUMBER: 141:7131

TITLE: Preparation of quinazolines and analogs as Akt

Searcher : Shears 571-272-2528

inhibitors and indoles as protein kinase inhibitors for use in synergistic combination therapy for the treatment of cancer

INVENTOR(S): Barnett, Stanley F.; Defeo-Jones, Deborah D.; Hartman, George D.; Huber, Hans E.; Stirdivant, Steven M.; Heimbrook, David C.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 121 pp., which
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004102360	A1	20040527	US 2003-678565	20031003
PRIORITY APPLN. INFO.:			US 2002-422312P	P 20021030
			US 2003-460911P	P 20030407

OTHER SOURCE(S): MARPAT 141:7131

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention relates to methods of treating cancer using a combination of at least two Akt inhibitors I [wherein Q = (un)substituted heterocyclyl, aryl; U, V, W, and X = independently CH, N; Y, Z = independently CH, N, provided that at least one of Y and Z = N; n = 0-3; p = 0-2; q = 0-4; R1, R2, R7 = independently halo, CN, OH, CHO, NO2, or (un)substituted (cyclo)alkyl(oxy), alkenyl(oxy), alkynyl(oxy), heterocyclyl(oxy), acyl, carboxy, carbamoyl(oxy), ureido, sulfamoyl, etc.; R3, R4 = independently H, (perfluoro)alkyl; or CR3R4 = cycloalkyl, heterocyclyl; and pharmaceutically acceptable salts or stereoisomers thereof] or a combination of I and a protein kinase inhibitor II [wherein G = H2, O; X = C, N, SO0-2, O; m = 0-2; n = 0-2; p = 0-6; q = 0-4; R1 = independently H, halo, or (un)substituted (cyclo)alkyl, heterocyclyl, aryl, carbamoyl, amino, acyl, sulfamoyl, carboxy, etc.; R2 = H or (un)substituted (cyclo)alkyl(oxy), amino, aryloxy, heterocyclyloxy, alkenyloxy, alkynyloxy, etc.; R5 = independently H, halo, NO2, CN, or (un)substituted alkyl, alkenyl, alkynyl, carboxy, acyl, sulfamoyl, carbamoyl, ureido, amino, etc.; and pharmaceutically acceptable salts or stereoisomers thereof], optionally in combination with a third compound. Examples include syntheses for I and II and assays demonstrating Akt inhibitor activity, antitumor activity, and the synergistic effect of combinations of AKT inhibitors and/or protein kinase inhibitors on caspase 3 activity. For instance, III•HCl was prepared in an 8-step reaction sequence culminating with the cycloaddn. of 4-(2-aminoprop-2-yl)benzil and o-phenylenediamine using glacial acetic acid in H2O, followed by work up with chloroform and ethanolic HCl. III•HCl, a selective Akt1 and Akt2 inhibitor, demonstrated a 3.2-fold in caspase 3 activation over control compared to a 1.2-fold increase for a protein kinase inhibitor. Combination treatment produced a 9-fold increase in caspase 3 activation.

IT 612847-29-7P 612848-47-2P

10/088814

RL: PAC (Pharmacological activity); RCT (Reactant);
SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
study); PREP (Preparation); RACT (Reactant or reagent); USES
(Uses)

(antitumor agent; preparation of quinazolines and analogs as Akt
inhibitors
and indoles as protein kinase inhibitors for use in synergistic
combination therapy for treatment of cancer)

L22 ANSWER 6 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 27 May 2004

ACCESSION NUMBER: 2004:430796 CAPLUS

DOCUMENT NUMBER: 141:7139

TITLE: Preparation of indolylquinoxalinones for treating
hyperproliferative disorders and diseases associated
with angiogenesis

INVENTOR(S): Ladouceur, Gaetan H.; Bear, Brian; Bi, Cheng;
Brittelli, David R.; Burke, Michael J.; Chen, Gang;
Cook, James; Dumas, Jacques; Sibley, Robert; Turner,
Michael R.

PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA

SOURCE: PCT Int. Appl., 217 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

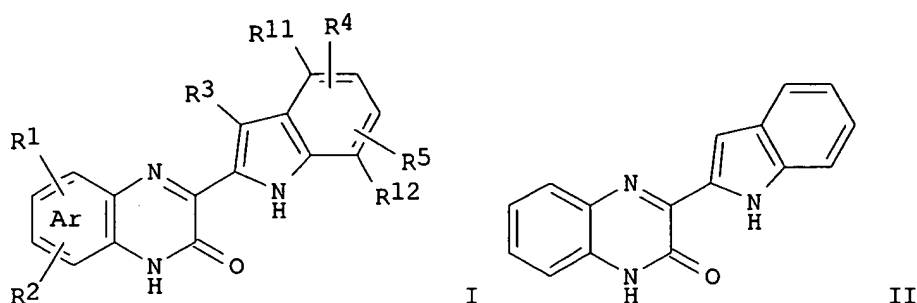
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004043950	A1	20040527	WO 2003-US36003	20031110
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,				
GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,				
LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,				
OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,				
TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,				
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,				
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,				
TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			US 2002-425490P	P 20021112
			US 2003-460915P	P 20030407
			US 2003-484202P	P 20030630

OTHER SOURCE(S): MARPAT 141:7139

GI



AB The invention relates to title compds. I [wherein Ar = 6-membered aromatic ring containing 0-2 N atoms; R1 and R2 = independently H, halo, CF₃, acyl, piperidinyl, piperazinyl, morpholinyl, or (un)substituted alkyl, alkoxy, amino, pyrrolidinyl, Ph, etc.; R3 = H, alkyl, OH, NO₂, NH₂, alkylamino, alkoxyamino, or (un)substituted benzoylamino; R4 = H, OH, halo, CN, acyl, sulfamoyl, trialkylsiloxy, tetrazolyl, thienyl, pyrrolyl, pyrimidinyl, oxazolyl, furanyl, or (un)substituted alkyl, alkenyl, alkynyl, alkoxy, amino, oxadiazolyl, Ph, pyridyl(oxy), carbamoyl; R11 and R12 = independently H, F, or Cl with the proviso that when one of R11 and R12 = F or Cl, the other must be H; and pharmaceutically acceptable salts and esters thereof]. The invention also relates to the use of I and their pharmaceutical compns. for treating hyperproliferative disorders and diseases associated with angiogenesis (no data). Examples include representative syntheses for compds. of the invention, pharmaceutical compns. comprising them, and tumor model assays (no specific data given). For instance, N-Boc-indole was coupled with di-Me oxalate using t-BuLi to give tert-Bu 2-[methoxy(oxo)acetyl]-1H-indole-1-carboxylate (72%). Cyclization of the dione with 1,2-phenylenediamine in AcOH afforded the quinoxalinone II (77%).

IT 694528-79-5P 694528-80-8P 694528-84-2P
 694528-95-5P 694528-97-7P 694529-00-5P
 694529-55-0P 694530-66-0P 694531-07-2P
 694531-12-9P 694531-13-0P 694531-15-2P
 694531-18-5P 694531-20-9P 694531-42-5P
 694532-17-7P 694532-22-4P

RL: PAC (Pharmacological activity); RCT (Reactant);
 SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(antiproliferative and angiogenesis inhibitor; preparation of indolylquinoxalinones for treating hyperproliferative disorders and diseases associated with angiogenesis)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 7 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 21 May 2004

ACCESSION NUMBER: 2004:412920 CAPLUS

DOCUMENT NUMBER: 140:423590

TITLE: Preparation of 4-(phenylpiperidin-4-ylidenemethyl)benzamides for treatment of pain,

anxiety, or gastrointestinal disorders
 INVENTOR(S): Brown, William; Griffin, Andrew
 PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
 SOURCE: PCT Int. Appl., 96 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041784	A1	20040521	WO 2003-SE1705	20031105
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			SE 2002-3301	A 20021107
OTHER SOURCE(S):		MARPAT 140:423590		
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [wherein R1 = (un)substituted alkyl, cycloalkyl(alkyl), (hetero)aryl, R8CO, R8SO2, R8SO, R8NHCO, R8CS, or R8NHCS; ; R2 = H or (un)substituted alkyl; R3 = H or (un)substituted alkoxy carbonyl, alkyl, or cycloalkyl(alkyl); R8 = (un)substituted alkyl, (hetero)aryl(alkyl), or cycloalkyl(alkyl); or pharmaceutically acceptable salts thereof] were prepared as opioid δ receptor ligands. For example, reaction of 4-(bromomethyl)benzoic acid Me ester with P(OMe)3, followed by addition of 1-(tert-butoxycarbonyl)-4-piperidone in the presence of LDA in THF, gave 4-(4-methoxycarbonylbenzylidene)piperidine-1-carboxylic acid tert-Bu ester (35%). Addition of Br2 (78%) and reaction with NaOH in MeOH provided 4-[bromo(4-carboxyphenyl)methylene]piperidine-1-carboxylic acid tert-Bu ester (87%). Conversion to the benzoyl chloride with iso-Bu chloroformate and amidation (73%) with Et2NH in the presence of TEA in CH2Cl2, followed by coupling with 3-aminophenylboronic acid using Pd(PPh3)4 and Na2CO3 in toluene/EtOH/H2O afforded N,N-diethyl-4-[(3-aminophenyl)(piperidin-4-ylidene)methyl]benzamide (97%). Alkylation of the amine with benzaldehyde and NaBH(OAc)3 in 1,2-dichloroethane gave II. In binding assays using human 293S cells expressing cloned human opioid receptors and neomycin resistance, most compds. of the invention exhibited activity toward the δ receptor with IC50 values in the range of 0.14 nM - 31.2 nM. Exemplified compds. also showed some activity toward the κ and μ receptors with IC50 values in the ranges of 36 nM - 9680 nM and 3 nM - 5975 nM, resp. Thus, I and their pharmaceutical compns. are useful in therapy, in particular for the treatment of gastrointestinal disorders,

anxiety, or pain (no data).
 IT 692246-95-0P
 RL: PAC (Pharmacological activity); RCT (Reactant);
 SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
 study); PREP (Preparation); RACT (Reactant or reagent); USES
 (Uses)
 (δ receptor agonist; preparation of (phenylpiperidinylidenemethyl)benz
 amides as δ receptor agonists for treatment of pain, anxiety, or
 gastrointestinal disorders)

L22 ANSWER 8 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 13 May 2004

ACCESSION NUMBER: 2004:390233 CAPLUS

DOCUMENT NUMBER: 140:406822

TITLE: A preparation of heteroaryl-hexanoic acid amide
 derivatives as immunomodulatory agents

INVENTOR(S): Brown, Matthew Frank; Gaweco, Anderson See; Gladue,
 Ronald Paul; Kath, John Charles; Poss, Christopher
 Stanley

PATENT ASSIGNEE(S): Pfizer Products Inc., USA

SOURCE: PCT Int. Appl., 66 pp.

CODEN: PIXXD2

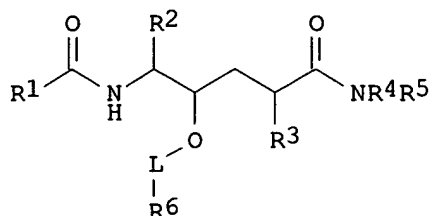
DOCUMENT TYPE: Patent

LANGUAGE: English

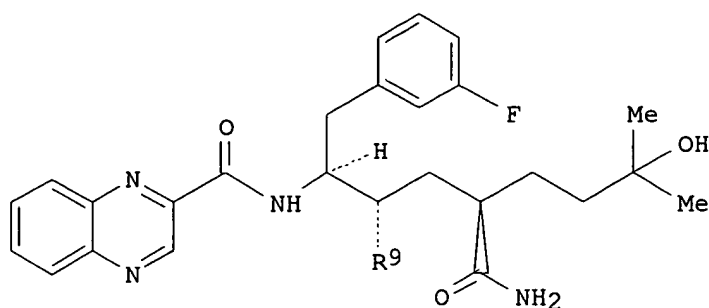
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004039787	A1	20040513	WO 2003-IB4626	20031020
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,				
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,				
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,				
PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,				
TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,				
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,				
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,				
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004097554	A1	20040520	US 2003-687380	20031016
PRIORITY APPLN. INFO.:			US 2002-422574P	P 20021030
OTHER SOURCE(S):	MARPAT	140:406822		
GI				



I



II

AB The invention relates to heteroaryl-hexanoic acid amide derivs. of formula I [wherein: R1 is a substituted heteroaryl; R2 is phenyl-(CH2)0-4, naphthyl-(CH2)0-4, or C3-C10cycloalkyl-(CH2)0-4, etc.; R3 is H, C1-10alkyl, C3-C10cycloalkyl-(CH2)0-6, (hetero)aryl-(CH2)0-6; R4 is H, alkyl, OH, alkoxy, hydroxyalkyl, alkoxy-C(O)-, etc.; R5 is H, alkyl, or amino; R4 and R5 together with the N-atom to which they are attached form (un)substituted C2-C9heterocycloalkyl; R6 is H, (HO)2P(O)-, HOS(O)2-, etc.; L is a bond or -O(CR7R8)-; R7 and R8 are independently H or C1-C3alkyl], useful as immunomodulatory agents. The invented compds. are inhibiting cell infiltration (ED50 < 30 μ M). The proposed dose of the invented compds. for oral, parenteral, nasal, or buccal administration to the average adult human is 0.1 to 1 g per unit dose. The invention relates

to

methods of using the above-described compds. and compns. for the treatment and prevention of diseases and conditions including those that may be treated or prevented by antagonizing the CCR1 receptor. For instance, hexanoic acid amide derivative II [R9 = OC(O)(CH2)2CO2H] was prepared via esterification of succinic anhydride by alc. II (R9 = OH).

IT **91-19-ODP**, Quinoxaline, derivs.

RL: **PAC (Pharmacological activity); RCT (Reactant);**

SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent); USES** (Uses)

(preparation of heteroaryl-hexanoic acid amide derivs. useful as immunomodulatory agents)

L22 ANSWER 9 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 28 Apr 2004

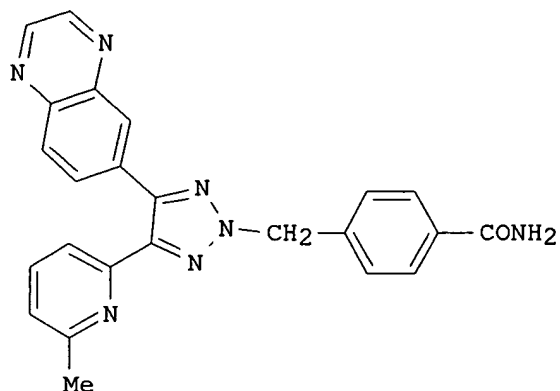
ACCESSION NUMBER: 2004:346231 CAPLUS

DOCUMENT NUMBER: 141:71490

TITLE: Synthesis and biological evaluation of novel

10/088814

AUTHOR(S): 2-pyridinyl-[1,2,3]triazoles as inhibitors of transforming growth factor β 1 type 1 receptor
Kim, Dae-Kee; Kim, Joonseop; Park, Hyun-Ju
CORPORATE SOURCE: College of Pharmacy, Ewha Womans University, 11-1 Daehyun-dong, Seodaemun-gu, Seoul, 120-750, S. Korea
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(10), 2401-2405
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:71490
GI



I

AB A series of 2-pyridinyl-[1,2,3]triazoles have been synthesized and evaluated for their ALK5 inhibitory activity in the luciferase reporter assays. Quinoxalinylnyl-substituted 2-pyridinyl-[1,2,3]triazole I showed significant ALK5 inhibition (SBE-luciferase activity, 25%; p3TP-luciferase activity, 17%) at a concentration of 5 μ M that is comparable to that of SB-431542 (SBE-luciferase activity, 21%; p3TP-luciferase activity, 12%), but weak p38 α MAP kinase inhibition (13%) at a concentration of 10 μ M that is much lower than that of SB-431542 (54%).

IT 710946-98-8P 710946-99-9P 710947-10-7P

RL: PAC (Pharmacological activity); RCT (Reactant);

SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation);

RACT (Reactant or reagent)

(preparation of 2-pyridinyl-[1,2,3]triazoles as inhibitors of transforming

growth factor β 1 type 1 receptor)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 10 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 15 Apr 2004

ACCESSION NUMBER: 2004:306973 CAPLUS

DOCUMENT NUMBER: 141:33319

Searcher : Shears 571-272-2528

10/088814

TITLE: Design, synthesis, and biological evaluation of novel 2-pyridinyl-[1,2,4]triazoles as inhibitors of transforming growth factor β 1 type 1 receptor

AUTHOR(S): Kim, Dae-Kee; Kim, Joonseop; Park, Hyun-Ju

CORPORATE SOURCE: College of Pharmacy, Ewha Womans University, Seoul, 120-750, S. Korea

SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(9), 2013-2020
CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of 2-pyridinyl-[1,2,4]triazoles have been synthesized and evaluated for their ALK5 inhibitory activity in the luciferase reporter assays. Compound 12b showed significant ALK5 inhibition (SBE-Luciferase, 73%; p3TP-Luciferase, 85%) at a concentration of 5 μ M that is comparable to that of SB-431542 (SBE-Luciferase, 79%; p3TP-Luciferase, 88%), but weak p38 α MAP kinase inhibition (4%) at a concentration of 10 μ M that is much lower than that of SB-431542 (54%). The binding mode of 12b generated by flexible docking studies revealed that the structure of 12b is a good fit into the (NPC-30345)-binding cavity of ALK5.

IT 701979-18-2P 701979-19-3P
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(design, synthesis, and biol. evaluation of novel 2-pyridinyl-[1,2,4]triazoles as inhibitors of transforming growth factor β 1 type 1 receptor)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 11 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 02 Mar 2004

ACCESSION NUMBER: 2004:168613 CAPLUS

DOCUMENT NUMBER: 140:368093

TITLE: A New Series of Highly Potent Non-Peptide Bradykinin B2 Receptor Antagonists Incorporating the 4-Heteroarylquinoline Framework. Improvement of Aqueous Solubility and New Insights into Species Difference

AUTHOR(S): Sawada, Yuki; Kayakiri, Hiroshi; Abe, Yoshito; Imai, Keisuke; Mizutani, Tsuyoshi; Inamura, Noriaki; Asano, Masayuki; Aramori, Ichiro; Hatori, Chie; Katayama, Akira; Oku, Teruo; Tanaka, Hirokazu

CORPORATE SOURCE: Exploratory Research Laboratories, Fujisawa Pharmaceutical Co. Ltd., Ibaraki, 300-2698, Japan

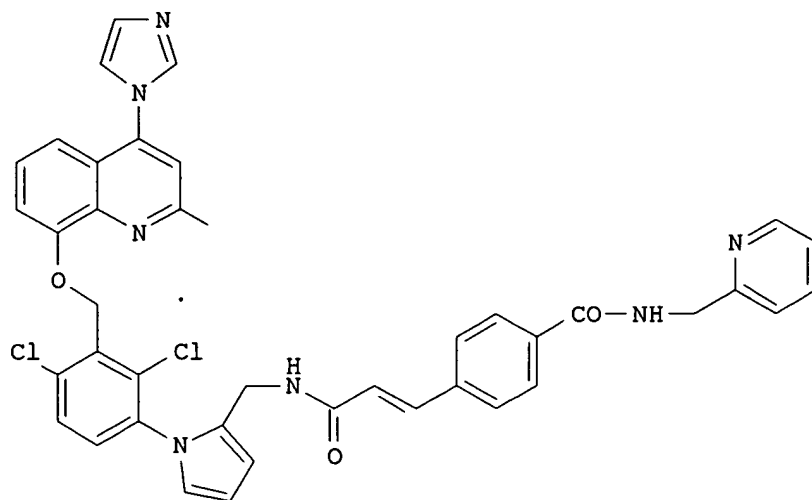
SOURCE: Journal of Medicinal Chemistry (2004), 47(7), 1617-1630
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB Introduction of nitrogen-containing heteroarom. groups at the 4-position of the quinoline moiety of the authors non-peptide B2 receptor antagonists resulted in enhancing binding affinities for the human B2 receptor and reducing binding affinities for the guinea pig one, providing new structural insights into species difference. A CoMFA study focused on the diversity of the quinoline moiety afforded correlative and predictive QSAR models of binding for the human B2 receptor but not for the guinea pig one. A series of 4-(1-imidazolyl)quinoline derivs. could be dissolved in a 5% aqueous solution of citric acid up to a concentration of 10 mg/mL. A representative compound (I) inhibited the specific binding of [³H]bradykinin to the cloned human B2 receptor expressed in Chinese hamster ovary cells with an IC₅₀ value of 0.26 nM and significantly inhibited bradykinin-induced bronchoconstriction in guinea pigs even at 1 µg/kg by i.v. administration.

IT 215238-12-3 683273-27-0

RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(bradykinin B2 receptor antagonists incorporating the 4-heteroarylquinoline framework and improvement of aqueous solubility and new insights into species difference in relation to bronchodilating activity)

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

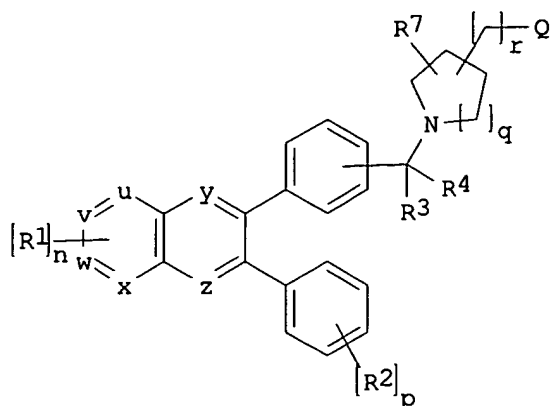
L22 ANSWER 12 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 29 Feb 2004

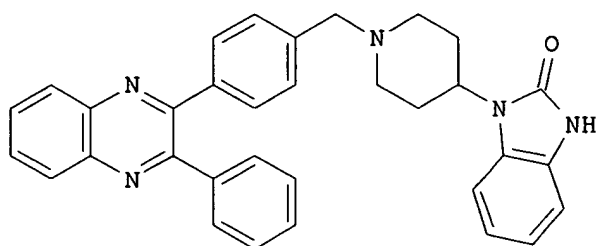
ACCESSION NUMBER: 2004:162686 CAPLUS

DOCUMENT NUMBER: 140:199493

TITLE: Preparation of novel quinuclidine derivatives for therapeutic use in the treatment of diseases or disorders responsive to modulation of cholinergic receptors and/or monoamine receptors



I



II

AB The title compds. comprising a 2,3-diphenylquinoxaline moiety [I; u, v, w and x = CH, N; y, z = CH, N (provided that at least one of y and z = N); Q = NR₅R₆, (un)substituted aryl, heterocyclyl; R₁ = alkenyl, halo, CN, etc.; R₂ = OH, CN, CO₂H, etc.; R₃, R₄ = H, alkyl, perfluoroalkyl; or R₃ and R₄ are combined to form (CH₂)_t wherein one of the carbon atoms is optionally replaced by O, SO_m, (un)substituted NHCO, N(COH); R₅, R₆ = H, aryl, heterocyclyl, etc.; or NR₅R₆ = monocyclic or bicyclic heterocycle; R₇ = halo, CN, CO₂H, etc.; n = 0-3; p = 0-2; t = 2-6; m = 0-2; q = 0-4; r = 0-1] and their salts which inhibit the activity of Akt, a serine/threonine protein kinase, were prepared. E.g., a 2-step synthesis of the quinoxaline II [starting from 4-bromomethylbenzil and 4-(2-keto-1-benzimidazolyl)piperidine], was given. The exemplified compds. I were found to have IC₅₀ of ≤ 50 μM against one or more of Akt1, Akt2 and Akt3. The invention is further directed to chemotherapeutic compns. containing the compds. I and methods for treating cancer comprising administration of the compds. I.

IT 612847-29-7P 612847-31-1P 612848-75-6P
612848-76-7P

RL: PAC (Pharmacological activity); RCT (Reactant);
SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES
(Uses)

(preparation of 2,3-diphenylquinoxaline derivs. as inhibitors of Akt activity for treating cancer)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 20 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 17 Oct 2003

ACCESSION NUMBER: 2003:818232 CAPLUS

DOCUMENT NUMBER: 139:323527

TITLE: Preparation of triazolo[4,3-b]pyridazines and 2,3-diarylquinazolines for the treatment of cancer
 INVENTOR(S): Barnett, Stanley F.; Defeo-Jones, Deborah; Haskell, Kathleen M.; Huber, Hans E.; Nahas, Deborah D.; Lindsley, Craig W.; Zhao, Zhijian; Hartman, George D.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 170 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

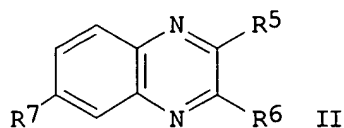
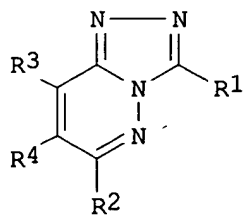
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003084473	A2	20031016	WO 2003-US10632	20030404
WO 2003084473	A3	20040212		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-370827P P 20020408
 US 2002-417202P P 20021009

GI



AB Triazolo[4,3-b]pyridazines I [R1 = (un)substituted Ph, furyl, thienyl, pyridinyl; R2 = substituted NH2, OH; R3 = H, R4 = (un)substituted cycloalkyl, aryl; R3R4 = (un)substituted CH:CHCH:CH] and quinazolines II [R5, R6 = (un)substituted Ph; R7 = H, alkyl, halogen, OH, alkoxy] were prepared for use as inhibitors of one or two of the isoforms of Akt, a serine/threonine protein kinase, acting particularly on the pleckstrin homol. domain of Akt. Thus, 3,6-dichloropyridazine was converted to its

4-cyclobutyl derivative which was cyclized with BzNHNH2 and aminated to give I
[R1 = Ph, R2 = NHCH2CMe2CH2NMe2, R3 = H, R4 = cyclobutyl]. This compound had IC50 for inhibition of Akt1 of 1.4 μ M.

IT 612847-30-0P 612847-32-2P

RL: PAC (Pharmacological activity); RCT (Reactant);
SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES
(Uses)

(preparation of triazolo[4,3-b]pyridazines and 2,3-diarylquinazolines for the treatment of cancer)

L22 ANSWER 21 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 26 Aug 2003

ACCESSION NUMBER: 2003:665554 CAPLUS

DOCUMENT NUMBER: 139:285655

TITLE: Potent quinoxaline-based inhibitors of PDGF receptor tyrosine kinase activity. Part 2: the synthesis and biological activities of RPR127963, an orally bioavailable inhibitor

AUTHOR(S): He, Wei; Myers, Michael R.; Hanney, Barbara; Spada, Alfred P.; Bilder, Glenda; Galzinski, Helen; Amin, Dilip; Needle, Saul; Page, Ken; Jayyosi, Zaid; Perrone, Mark H.

CORPORATE SOURCE: Aventis Pharmaceuticals, Bridgewater, NJ, 08807, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(18), 3097-3100

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:285655

AB RPR127963 demonstrates an excellent pharmacokinetic profile in several species and was found to be efficacious in the prevention of restenosis in a Yucatan mini-pig model upon oral administration of 1-5 mg/kg. The in vitro selectivity profile and SAR of the highly optimized PDGF-R tyrosine kinase inhibitor are highlighted.

IT 217093-53-3P

RL: PAC (Pharmacological activity); RCT (Reactant);
SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES
(Uses)

(synthesis and PDGF receptor tyrosine kinase-inhibiting activity of RPR127963 and its derivs.)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 22 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 01 Aug 2003

ACCESSION NUMBER: 2003:591177 CAPLUS

DOCUMENT NUMBER: 139:149652

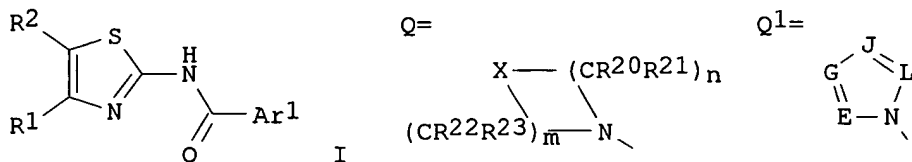
TITLE: Preparation of 2-acylaminothiazole derivatives or salts thereof as c-Mpl receptor ligands

INVENTOR(S): Sugasawa, Keizo; Watanuki, Susumu; Koga, Yuji; Nagata, Hiroshi; Obitsu, Kazuyoshi; Wakayama, Ryutaro; Hirayama, Fukushima; Suzuki, Ken-ichi

10/088814

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 110 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003062233	A1	20030731	WO 2003-JP270	20030115
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG EP 1466912 A1 20041013 EP 2003-700571 20030115 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK PRIORITY APPLN. INFO.: JP 2002-10413 A 20020118 JP 2002-10447 A 20020118 WO 2003-JP270 W 20030115 OTHER SOURCE(S): MARPAT 139:149652 GI				



AB 2-Acylaminothiazole derivs. or pharmaceutically acceptable salts thereof [I; Ar1 = each (un)substituted aryl, monocyclic aromatic heterocyclyl, or bicyclic condensed heterocyclyl; R1 = each (un)substituted aryl or monocyclic aromatic heterocyclyl; R2 = Q, Q1, R24R25N; wherein n, m = an integer of 1-3; when n or m is an integer of ≥ 2 , CR20R21 and CR22R23 may represent a different group; X = O, S, NR26, C(R27)R28; E, G, J, L = N, CR29; R20-R23, R26-R29 = H, OH, lower alkoxy, each (un)substituted lower alkyl, cycloalkyl, aryl, arylalkyl, aromatic heterocyclyl, aromatic heterocyclylalkyl, nonarom. heterocyclyl, lower alkenyl, lower alkylidene, NH2, or CONH2, CO2H, lower alkoxy, lower alkenyloxycarbonyl, aryl-lower alkoxy, aromatic heterocyclyl-lower alkoxy, lower alkylcarbonylamino, oxo; R24, R25 = H, each (un)substituted lower alkyl, cycloalkyl, or nonarom. heterocyclyl] are prepared. These compds. have an excellent effect of proliferating human c-Mpl-Ba/F3 cells and an activity of increasing platelets (thrombocytosis) based on the effect of promoting the formation

of megakaryocytic colonies and are useful in treating thrombopenia. Thus, 2.1 mL Et isonipecotinate was added to a solution of 750 mg 5,6-dichloro-N-[4-(4-chlorothiophen-2-yl)-5-(4-cyclohexylpiperazin-1-yl)thiazol-2-yl]nicotinamide in 10 mL THF, heated to 50°, and stirred for 5 h to give, after workup and silica gel chromatog., 881 mg 1-[3-chloro-5-[[4-(4-chlorothiophen-2-yl)-5-(4-cyclohexylpiperazin-1-yl)thiazol-2-yl]carbamoyl]-2-pyridyl]piperidine-4-carboxylic acid Et ester which (30 mg) was dissolved in 1 mL MeOH, treated with 0.12 mL 1 M aqueous NaOH solution at room temperature, stirred for 24 h, distilled under reduced pressure, dissolved in EtOAc, treated with 0.2 mL 1 M aqueous HCl solution, stirred, and distilled under reduced pressure, followed by washing the residue with Et2O to give 20 mg 1-[3-chloro-5-[[4-(4-chlorothiophen-2-yl)-5-(4-cyclohexylpiperazin-1-yl)thiazol-2-yl]carbamoyl]-2-pyridyl]piperidine-4-carboxylic acid hydrochloride (II). II and recombinant human thrombopoietin (rhTPO) at 2.4 ad 0.012 nM, resp., showed 30% of the maximum cell proliferating effect of each compound tested on human c-Mpl-Ba/F3 cell.

IT **570405-07-1P**
 RL: **PAC (Pharmacological activity); RCT (Reactant);**
 SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent);** USES (Uses)
 (preparation of 2-acylaminothiazole derivs. or salts thereof as c-Mpl receptor ligands for proliferating human c-Mpl-Ba/F3 cells and increasing platelets via promoting the formation of megakaryocytic colony)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 23 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 30 May 2003

ACCESSION NUMBER: 2003:412773 CAPLUS

DOCUMENT NUMBER: 139:381448

TITLE: Some reactions with ketene dithioacetals. Part II: Novel synthesis of quinoxaline, pyrazole and pyrrolo[3,4-b]quinoxaline derivatives using ketene dithioacetals as antimicrobial activity

AUTHOR(S): El-Sharief, A. M. Sh.; Zahran, M. A.; El-Gaby, M. S. A.; Ammar, Y. A.; El-Said, U. H.

CORPORATE SOURCE: Chemistry Department, Faculty of Science, Al-Azhar University, Nasr City, Cairo, Egypt

SOURCE: Afinidad (2003), 60(503), 81-87

CODEN: AFINAE; ISSN: 0001-9704

PUBLISHER: Asociacion de Quimicos del Instituto Quimico de Sarria

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:381448

AB The key compound, [(4-aminophenylaminomethylthio)methylene]malonitrile (I) was synthesized by condensation of ketene dithioacetals and 1,4-phenylenediamine. The reactivity of quinoxaline-2,3-dicarboxylic anhydride (II) towards compound I as nitrogen nucleophile was investigated. Thus, treatment of compound II with I in refluxing ethanol afforded the quinoxaline carboxylic acid derivative (III). On the other hand, fusion of compound II and I at 160°C yielded the corresponding quinoxaline carboxamide (IV). Fusion of compds. III and IV with hydrazine hydrate at

150°C produced the novel corresponding substituted pyrazoles. Refluxing of compound III with acetic anhydride furnished the novel pyrrolo[3,4-b]quinoxaline. By treatment of compound I with aromatic sulfonyl chloride followed by fusion with hydrazine, the novel pyrazole was obtained. The anti-microbial activity of some selected compound was also reported.

IT 623934-58-7P 623934-59-8P

RL: PAC (Pharmacological activity); RCT (Reactant);

SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation);

RACT (Reactant or reagent)

(ring closure of; multi-step preparation of quinoxaline, pyrazole and pyrroloquinoxaline derivs. using ketene dithioacetals and their antimicrobial activity)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 24 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 07 Mar 2003

ACCESSION NUMBER: 2003:174477 CAPLUS

DOCUMENT NUMBER: 138:226731

TITLE: Alpha-2-adrenergic agonist/fatty acid compositions

INVENTOR(S): Woodward, David F.; Ambrus, Gyorgy

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 13 pp., Cont.-in-part of U.S. Pat. Appl. 2002 198,210.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003045524	A1	20030306	US 2002-136263	20020501
US 2002198210	A1	20021226	US 2001-848249	20010503
PRIORITY APPLN. INFO.:			US 2001-848249	A2 20010503

AB Compns. comprising an alpha-2-adrenergic agonist component and a fatty acid component, that enhances the pharmacokinetic disposition of the therapeutic component, are disclosed. The fatty acid component may include linolenic acid and/or other fatty acids. A brimonidine-linoleic acid complex was formed and its effect on intraocular pressure determined

IT 59803-98-4, Brimonidine 91147-43-2, 6-Quinoxalinamine, N-(4,5-dihydro-1H-imidazol-2-yl)- 474777-33-8

RL: PAC (Pharmacological activity); RCT (Reactant);

THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(α2-adrenergic agonist/fatty acid compns.)

L22 ANSWER 25 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 07 Feb 2003

ACCESSION NUMBER: 2003:97401 CAPLUS

DOCUMENT NUMBER: 138:153554

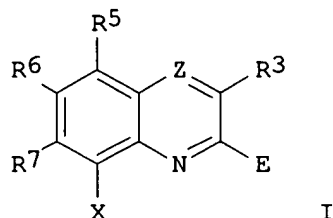
TITLE: Preparation of quinoline and quinoxaline derivatives as inhibitors of factor Xa with therapeutic uses

INVENTOR(S): Schmitt, Martine; Klotz, Evelyne; Macher, Jean-Paul;

10/088814

PATENT ASSIGNEE(S): Bourguignon, Jean-Jacques
 SOURCE: NEURO3D, Fr.
 PCT Int. Appl., 283 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003010146	A1	20030206	WO 2002-FR2594	20020719
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
FR 2827599	A1	20030124	FR 2001-9730	20010720
EP 1451159	A1	20040901	EP 2002-790206	20020719
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
PRIORITY APPLN. INFO.:			FR 2001-9730	A 20010720
			WO 2002-FR2594	W 20020719
OTHER SOURCE(S):			MARPAT 138:153554	
GI				



AB The invention concerns compds. quinoline and quinoxaline derivs. (shown as I; variables defined below; e.g. 4,8-dihydroxy-5,7-dichloroquinoline-2-carboxylic acid), their preparation and their uses, in particular in therapeutic treatments and vaccines or for developing active compds. For I: E = COOH, COOR1, CH2OH, CHO, CH2COOH, CH2COOR1, C(O)NHR2, or 1H-tetrazol-5-yl; R1 = (C1-C12)alkyl or (C6-C18)aryl(C1-C12)alkyl; R2 = H, (C1-C12)alkyl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl, hydroxy; R3 = H, halo, hydroxy, (C1-C12)alkyl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl or (C3-C17)heteroaryl. Z = N or CR4; R4 = H, (C1-C12)alkyl, (C2-C12)alkyn-1-yl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl, OR8, NR9R9, (C1-C17)heteroaryl or (C2-C12)alken-1-yl; R5, R6 and R7 = H, halo, (C1-C12)alkyl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl, NR9R9', COR10, (C2-C12)alken-1-yl, (C2-C12)alkyn-1-yl, (C1-C17)heteroaryl, (C3-C17)heteroaryl(C1-C12)alkyl, cyano or nitro; -R8 = H, (C1-C12)alkyl,

Searcher : Shears 571-272-2528

(C6-C18)aryl(C1-C12)alkyl. R9 = H, (C1-C12)alkyl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl, acyl, tert-butoxycarbonyl, (C1-C17)heteroaryl or (C6-C18)arylsulfonyl or (C1-C12)alkylsulfonyl; R9', which may be same or different than R9 = H, (C1-C12)alkyl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl, acyl, tert-butoxycarbonyl, (C1-C17)heteroaryl or (C6-C18)arylsulfonyl or (C1-C12)alkylsulfonyl; NR9R9' = cycloheteroalkyl: N(CH₂)_m(CH₂)_nY (n = 2 or 3, m = 2 or 3 and Y = CH₂, SO₂, or NR11, O, S); R10 = H, (C1-C12)alkyl or (C6-C18)aryl or NHR2. R11 = H, (C1-C12)alkyl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl, (C1-C17)heteroaryl, (C1-C17)heteroaryl(C1-C12)alkyl or COR10; X = halo, OR8, NR9R9', (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl, (C3-C12)alkyl, (C2-C12)alken-1-yl, (C2-C12)alkyn-1-yl, (C1-C17)heteroaryl, COR10, cyano or nitro; addnl. details are given in the claims. Test results for inhibition of factor Xa by .apprx.50 examples of I are included; for example, 4,8-dihydroxy-5,7-dichloroquinoline-2-carboxylic acid exhibits IC₅₀ = 4.6 μM and 163 % of the inhibitory activity of xanthurenic acid at 10 μM. More than 100 example preps. of I are included. For example, Me 4-hydroxy-6-bromo-8-methoxyquinoline-2-carboxylate was prepared in 64% yield from Me 2-[(4-bromo-2-methoxyphenyl)amino]but-2-enedioate in Ph₂O at 250° for 5-15 min; the reactant was prepared in 93% yield from 2-methoxy-4-bromoaniline and Me acetylenedicarboxylate in MeOH at reflux for 1 h.

IT **495407-42-6P**, Ethyl 8-hydroxy-3-oxo-3,4-dihydroquinoxaline-2-carboxylate **495407-43-7P**, Ethyl 8-(benzyloxy)-3-oxo-3,4-dihydroquinoxaline-2-carboxylate **495407-45-9P**, Ethyl [8-(benzyloxy)-3-oxo-3,4-dihydroquinoxaline-2(1H)-ylidene]acetate
 RL: **PAC (Pharmacological activity); RCT (Reactant);**
 SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent); USES**
 (Uses)

(drug candidate; preparation of quinoline and quinoxaline derivs. as inhibitors of factor Xa with therapeutic uses)

REFERENCE COUNT: 87 THERE ARE 87 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 26 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 11 Dec 2002

ACCESSION NUMBER: 2002:939992 CAPLUS

DOCUMENT NUMBER: 139:270356

TITLE: Comparative study of isoflavone, quinoxaline and oxindole families of anti-angiogenic agents

AUTHOR(S): Whatmore, Jacqueline L.; Swann, Elizabeth; Barraja, Paola; Newsome, Jeffery J.; Bunderson, Melisa; Beall, Howard D.; Tooke, John E.; Moody, Christopher J.

CORPORATE SOURCE: School of Sport and Health Sciences, University of Exeter, Exeter, EX4 4QD, UK

SOURCE: Angiogenesis (2002), 5(1-2), 45-51

CODEN: AGIOFT; ISSN: 0969-6970

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:270356

AB A study designed to compare the effects on VEGF-induced angiogenesis of a number of known anti-angiogenic agents together with some novel derivs. thereof was undertaken. Thus the isoflavone biochanin A (1), indomethacin (2), the 3-arylquinoxaline SU1433 and its derivs. (3-6), the benzoic acid

derivative (7), the oxindoles SU5416 (8) and SU6668 (11), together with their simple N-benzyl derivs. (9, 10, and 12) were selected for study. Using an in vitro assay the compds. were evaluated for their ability to inhibit VEGF-induced angiogenesis in HUVECs, and the cytotoxicity of representative compds. was also studied in tumor cell lines using 24-h exposure. The results indicate that the SU compds., SU1433, SU5416 and SU6668, are more potent inhibitors of VEGF-induced angiogenesis than indomethacin or the naturally occurring biochanin A, presumably because they inhibit VEGF receptor signaling. Blocking one of the phenolic OH groups of SU1433 reduced anti-angiogenic activity, as did blocking the NH groups of SU5416 and SU6668. Cytotoxicity studies indicate that none of the compds. examined exhibited cytotoxicity at anti-angiogenic concns.

IT 168835-90-3P, SU 1433

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation and comparative study of isoflavone, quinoxaline and oxindole

families of anti-angiogenic agents)

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 27 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 03 Dec 2002

ACCESSION NUMBER: 2002:917077 CAPLUS

DOCUMENT NUMBER: 139:36744

TITLE: A versatile synthetic route to chiral quinoxaline derivatives from amino acids precursors

AUTHOR(S): El-Faham, Ayman; El Massry, Abdel Moneim; Amer, Adel; Gohar, Yousry M.

CORPORATE SOURCE: Faculty of Science, Chemistry Department, University of Alexandria, Alexandria, Egypt

SOURCE: Letters in Peptide Science (2002), 9(1), 49-54
CODEN: LPSCEM; ISSN: 0929-5666

PUBLISHER: Kluwer Academic Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:36744

AB The synthesis of N-protected L-amino acid (3-benzylquinoxalin-2-yl)hydrazide derivs. is reported. 3-Benzyl-2-hydrazinoquinoxaline was prepared and then coupled with N-Boc-L-amino acids, including alanine, valine, leucine, phenylalanine, tyrosine, serine and proline, in the presence of HBTU as a coupling reagent to provide the expected product with high yield and purity. The products were deprotected by p-toluenesulfonic acid in acetonitrile and the tosylate salts were evaluated for antibacterial and antifungal activity.

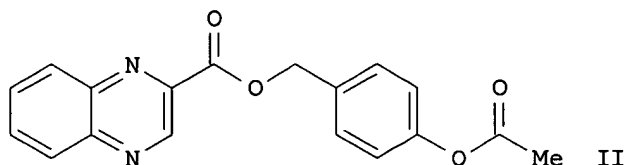
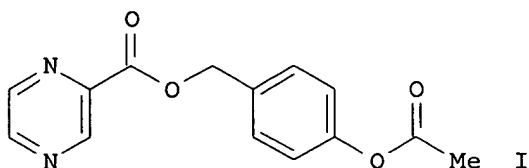
IT 223929-23-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of L-amino acid (benzylquinoxaliny)hydrazide derivs. and their antibacterial and antifungal activities)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 28 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
 ED Entered STN: 07 Nov 2002
 ACCESSION NUMBER: 2002:844381 CAPLUS
 DOCUMENT NUMBER: 138:73233
 TITLE: Synthesis and Antimycobacterial Activity of Pyrazine
 and Quinoxaline Derivatives
 AUTHOR(S): Seitz, Laine E.; Suling, William J.; Reynolds, Robert
 C.
 CORPORATE SOURCE: Organic Chemistry Department and Biochemistry
 Department, Southern Research Institute, Birmingham,
 AL, 35255-5305, USA
 SOURCE: Journal of Medicinal Chemistry (2002), 45(25),
 5604-5606
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:73233
 GI



AB A series of pyrazine and quinoxaline derivs. have been synthesized, and their activity against *M. tuberculosis* (Mtb) and *Mycobacterium avium* (MAC) are reported. The 4-acetoxymethyl ester of pyrazinoic acid (I) and 4'-acetoxymethyl 2-quinoxalinecarboxylate (II) showed excellent activity against Mtb (MIC ranges of less than 1-6.25 µg/mL) but only modest activity against MAC (MICs of 4-32 µg/mL).

IT 1865-11-8P

RL: PAC (Pharmacological activity); RCT (Reactant);
 SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation);
 RACT (Reactant or reagent)

(preparation, antitubercular activity, and structure-activity
 relationship
 of alkyl and benzyl quinoxalinecarboxylates via coupling of alcs. with
 quinoxalinecarbonyl chloride)

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REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 29 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 17 Oct 2002

ACCESSION NUMBER: 2002:790220 CAPLUS

DOCUMENT NUMBER: 137:294982

TITLE: Preparation of piperazinyldipyrzinyl aryloxyalkyl ethers as 5-HT_{2C} receptor agonists

INVENTOR(S): Nilsson, Bjorn; Tejbrant, Jan; Pelcman, Benjamin; Ringberg, Erik; Thor, Markus; Nilsson, Jonas; Jonsson, Mattias

PATENT ASSIGNEE(S): Biovitrum AB, Swed.

SOURCE: U.S., 45 pp., Cont.-in-part of U.S. Ser. No. 573,348, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

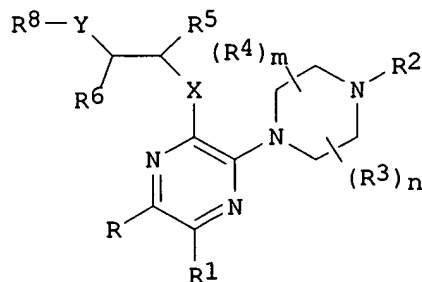
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

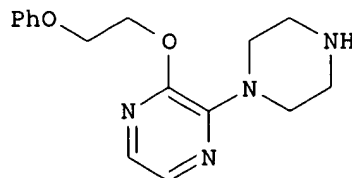
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6465467	B1	20021015	US 2000-589282	20000608
ZA 2001009571	A	20021120	ZA 2001-9571	20011120
US 2003092694	A1	20030515	US 2002-269670	20021011
US 6759401	B2	20040706		
US 2004242554	A1	20041202	US 2004-873852	20040622
PRIORITY APPLN. INFO.:			SE 1999-1884	A 19990521
			US 1999-137527P	P 19990603
			US 2000-573348	B2 20000519
			US 2000-589282	A3 20000608
			US 2002-269670	A1 20021011

OTHER SOURCE(S): MARPAT 137:294982
GI



I



II

AB The title compds. (I) [wherein X and Y = independently O, S, or NR₇; R and R₁ = independently H, alkyl, or halo; or C₂RR₁ = optionally halo substituted benzene or thiophene; R₂ = H, OH, or alkyl; R₃, R₄, and R₅ = independently H or alkyl; R₆ = H or alkyl; or CYR₆R₈ for a 5-6 membered heterocycle; R₇ = H or alkyl, preferably Me or Et; R₈ = (un)substituted (hetero)aryl; m and n = independently 1 or 2; or pharmaceutically

Searcher : Shears 571-272-2528

acceptable salts, hydrates, geometric isomers, tautomers, optical isomers, N-oxides, and prodrugs thereof] were prepared and tested as 5-HT_{2C} receptor agonists. For instance, 2,3-dichloropyrazine and 2-phenoxyethanol were treated with t-BuONa in dioxane to give 2-chloro-3-(2-phenoxyethoxy)pyrazine (62%). The halopyrazine, piperazine, and K₂CO₃ in MeCN were stirred and heated to afford the desired 2-(phenoxy)ethyl 3-(1-piperazinyl)-2-pyrazinyl ether (II) in 65% yield, which was then converted to the maleate salt. In competition expts., I showed affinity for 5-HT_{2C} receptor protein with K_i values typically ranging from 1 nM to 1500 nM and specific values ranging from 5 nM to 377 nM for twelve compds. I exhibited agonist efficacy at the 5-HT_{2C} receptor by mobilizing intracellular Ca in transfected HEK293 cells with maximum responses in the range of 20-100% relative to the maximum response of 5-HT (serotonin) at a concentration of 1 µM. Acute toxicity studies in mice following oral administration of I showed that mortality typically occurred at doses between 200 mg/kg to 450 mg/kg body weight I are useful for the treatment

of

serotonin-related central nervous system disorders, such as eating disorders, memory disorders, schizophrenia, mood disorders, anxiety disorders, pain, sexual dysfunctions, and urinary disorders (no data).

IT

313654-02-3P, 2-(2-Phenoxyethoxy)-3-(1-piperazinyl)quinoxaline

313656-86-9P, 2-[2-(3-Pyridinyloxy)ethoxy]-3-(1-

piperazinyl)quinoxaline **313656-92-7P**, 2-[2-(3-Pyridinyloxy)ethoxy]-3-(1-piperazinyl)-6,7-dichloroquinoxaline

RL: **PAC (Pharmacological activity); RCT (Reactant);**

SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological

study); PREP (Preparation); **RACT (Reactant or reagent); USES**

(Uses)

(preparation of heterocyclylpyrazinyl aryloxyalkyl ether 5-HT_{2C} receptor agonists from aryloxyalkanols, halopyrazines, and heterocycles)

REFERENCE COUNT:

32

THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 30 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 29 Jul 2002

ACCESSION NUMBER: 2002:558411 CAPLUS

DOCUMENT NUMBER: 137:257239

TITLE: SAR by MS: A Ligand Based Technique for Drug Lead Discovery Against Structured RNA Targets

AUTHOR(S): Swayze, Eric E.; Jefferson, Elizabeth A.; Sannes-Lowery, Kristin A.; Blyn, Lawrence B.; Risen, Lisa M.; Arakawa, Satoshi; Osgood, Stephen A.; Hofstadler, Steven A.; Griffey, Richard H.

CORPORATE SOURCE: Ibis Therapeutics, A Division of Isis Pharmaceuticals Inc., Carlsbad, CA, 92008, USA

SOURCE: Journal of Medicinal Chemistry (2002), 45(18), 3816-3819

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:257239

AB A technique for lead discovery vs. RNA targets utilizing mass spectrometry (MS) screening methods is described. The structure-activity relationships (SAR) derived from assaying weak binding motifs allows the pharmacophores discovered to be elaborated via "SAR by MS" to higher affinity ligands.

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Application of this strategy to a subdomain of the 23S rRNA afforded a new class of compds. with functional activity.

IT 14121-55-2

RL: CST (Combinatorial study, unclassified); **PAC (Pharmacological activity)**; **RCT (Reactant)**; THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); **RACT (Reactant or reagent)**; USES (Uses)

(SAR by MS: ligand-based technique for drug lead discovery against structured RNA targets)

IT 462119-65-9P 462119-66-0P 462119-67-1P
462119-68-2P 462119-69-3P

RL: **PAC (Pharmacological activity)**; **RCT (Reactant)**;
SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)

(SAR by MS: ligand-based technique for drug lead discovery against structured RNA targets)

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 31 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 11 Apr 2002

ACCESSION NUMBER: 2002:271488 CAPLUS

DOCUMENT NUMBER: 137:78924

TITLE: Synthesis and antimicrobial activity of novel
furothienoquinoxalines, pyranothienoquinoxalines and
pyrimidopyranothienoquinoxalines

AUTHOR(S): Moustafa, Osama S.; El-Ossaily, Yasser A.

CORPORATE SOURCE: Chemistry Department, Faculty of Science, Assiut
University, Assiut, 71516, Egypt

SOURCE: Journal of the Chinese Chemical Society (Taipei,
Taiwan) (2002), 49(1), 107-112
CODEN: JCCTAC; ISSN: 0009-4536

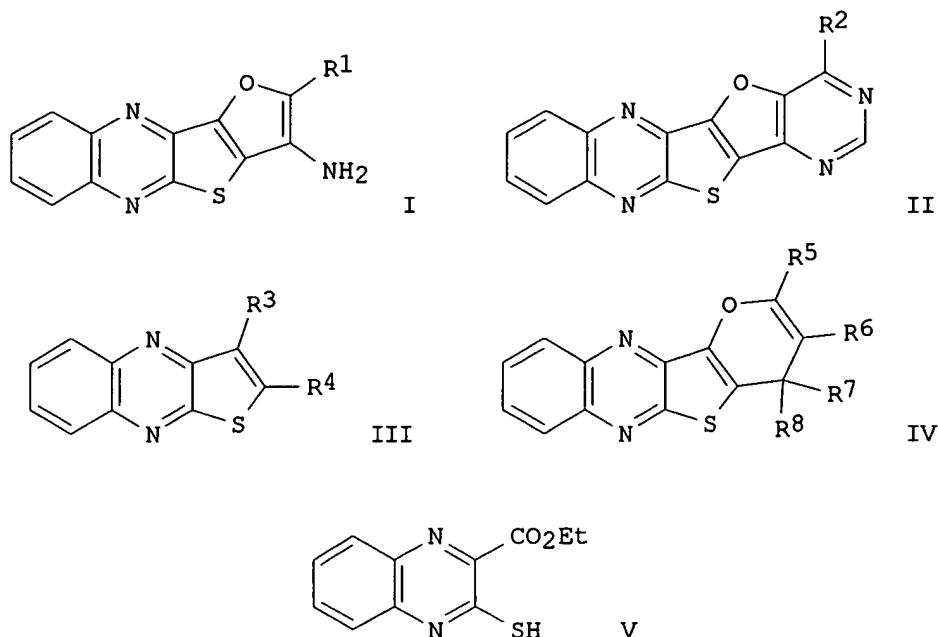
PUBLISHER: Chinese Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:78924

GI



AB Furothienoquinoxalines I (R¹ = CN, COOEt) and II (R² = HO, NH₂), thienoquinoxalines III (R³ = HO, EtO₂CCH₂O; R⁴ = H, CN), and pyranothienoquinoxalines IV (R⁵ = EtO₂C, EtO₂CCH:N, MeCONH; R⁶ = H, CN; R⁷ = Ph, R⁸ = H; R⁷R⁸ = O) were prepared by multi-step synthesis from mercaptoquinoxaline V and tested against Gram pos. and Gram neg. bacteria and fungi. Most of I-IV showed good growth inhibition against Gram pos. bacteria, while III (R³ = HO, R⁴ = H) was active against all types of bacteria and fungi studied.

IT 278186-19-9

RL: PAC (Pharmacological activity); RCT (Reactant);

BIOL (Biological study); RACT (Reactant or reagent)

(preparation of antibacterial and antifungal thienoquinoxalines via cyclocondensation of ethoxycarbonyl(mercapto)quinoxaline with α -halo ketones and esters)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 32 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 02 Apr 2002

ACCESSION NUMBER: 2002:246597 CAPLUS

DOCUMENT NUMBER: 137:134476

TITLE: Anti-Mycobacterium tuberculosis agents derived from quinoxaline-2-carbonitrile and quinoxaline-2-carbonitrile 1,4-di-N-oxide

AUTHOR(S): Ortega, Miguel Angel; Sainz, Yolanda; Montoya, Maria Elena; Jaso, Andres; Zarranz, Belen; Aldana, Ignacio; Monge, Antonio

CORPORATE SOURCE: Unidad en Investigacion y Desarrollo de Medicamentos, CIFA, Universidad de Navarra, Pamplona, Spain

SOURCE: Arzneimittel-Forschung (2002), 52(2), 113-119

10/088814

CODEN: ARZNAD; ISSN: 0004-4172
PUBLISHER: Editio Cantor Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:134476

AB In this paper new quinoxaline derivs. with different substituents in positions 3, 6, 7 and 8 are reported. Their biol. activities against Mycobacterium tuberculosis have been assessed and most of the 1,4-di-N-oxide derivs. have been shown to strongly inhibit the bacteria growth in the first in vitro screening. One of these N-oxides (4) is a promising candidate due to its good Selectivity Index (7.95). On the other hand, those compds. without N-oxide moieties showed no or very low activity (growth inhibition: 17% and 39%).

IT 444807-95-8P

RL: PAC (Pharmacological activity); RCT (Reactant);
SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES
(Uses)
(quinoxaline-2-carbonitrile derivs. anti-Mycobacterium tuberculosis action)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 33 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 20 Mar 2002

ACCESSION NUMBER: 2002:211240 CAPLUS

DOCUMENT NUMBER: 137:226178

TITLE: 5-Phosphonomethylquinoxalinediones as competitive NMDA receptor antagonists with a preference for the human 1A/2A, rather than 1A/2B receptor composition

AUTHOR(S): Auberson, Yves P.; Allgeier, Hans; Bischoff, Serge; Lingenhoehl, Kurt; Moretti, Robert; Schmutz, Markus

CORPORATE SOURCE: Novartis Pharma AG, Basel, 4002, Switz.

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(7), 1099-1102
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:226178

AB NMDA antagonists derived from 5-phosphonomethyl-1,4-dihydroquinoxaline-2,3-dione are potent anticonvulsant agents, and display strong protective effects in the electroshock-induced convulsion assay in mice. Their preference for the human NMDAR 1A/2A over 1A/2B subunit composition was optimized, leading to compound (1RS,1'S)-PEAQX, which shows a >100-fold selectivity.

IT 459836-14-7P 459836-15-8P

RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(5-phosphonomethylquinoxalinediones as competitive NMDA receptor antagonists with a preference for human 1A/2A, rather than 1A/2B receptor composition)

IT 187479-25-0 187479-26-1 459836-02-3
459836-07-8 459836-08-9 459836-09-0

Searcher : Shears 571-272-2528

10/088814

459836-22-7

RL: **PAC (Pharmacological activity)**; PRP (Properties); **RCT (Reactant)**; THU (Therapeutic use); BIOL (Biological study); **RACT (Reactant or reagent)**; USES (Uses)

(5-phosphonomethylquinoxalinediones as competitive NMDA receptor antagonists with a preference for human 1A/2A, rather than 1A/2B receptor composition)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 34 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 15 Feb 2002

ACCESSION NUMBER: 2002:119100 CAPLUS

DOCUMENT NUMBER: 138:83

TITLE: Quinoxaline chemistry. Part 14. 4-(2-Quinoxalylamino)-phenylacetates and 4-(2-quinoxalylamino)-phenylacetyl-l-glutamates as analogues-homologues of classical antifolate agents. Synthesis and evaluation of in vitro anticancer activity

AUTHOR(S): Piras, Sandra; Loriga, Mario; Paglietti, Giuseppe
CORPORATE SOURCE: Dipartimento Chimico Tossicologico, Universita di Sassari, Sassari, 07100, Italy

SOURCE: Farmaco (2002), 57(1), 1-8

CODEN: FRMCE8; ISSN: 0014-827X

PUBLISHER: Editions Scientifiques et Medicales Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:83

AB Among a new series of 26 4-(3-substituted-2-quinoxalylamino)phenylacetates and 4-(3-substituted-2-quinoxalylamino)phenylacetyl-l-glutamates, eight were selected at NCI for evaluation of their in vitro anticancer activity. The results obtained in comparison with the corresponding nor-compds. series seem to indicate that this type of homologation is not helpful.

IT 476374-02-4P 476374-03-5P 476374-04-6P

476374-05-7P 476374-06-8P 476374-07-9P

476374-08-0P 476374-09-1P 476374-10-4P

476374-11-5P 476374-12-6P 476374-13-7P

476374-14-8P 476374-15-9P 476374-16-0P

476374-17-1P 476374-18-2P 476374-27-3P

RL: DMA (Drug mechanism of action); **PAC (Pharmacological activity)**

; PRP (Properties); **RCT (Reactant)**; SPN (Synthetic preparation);

THU (Therapeutic use); BIOL (Biological study); PREP (Preparation);

RACT (Reactant or reagent); USES (Uses)

(quinoxaline chemical and synthesis and evaluation of in vitro anticancer activity)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 35 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 10 Feb 2002

ACCESSION NUMBER: 2002:107312 CAPLUS

DOCUMENT NUMBER: 136:167389

TITLE: Preparation of pyrrole, indole, thiophene, pyrazole, imidazole, and isothiazole derivatives as inhibitors of transforming growth factor-beta (TGF- β)

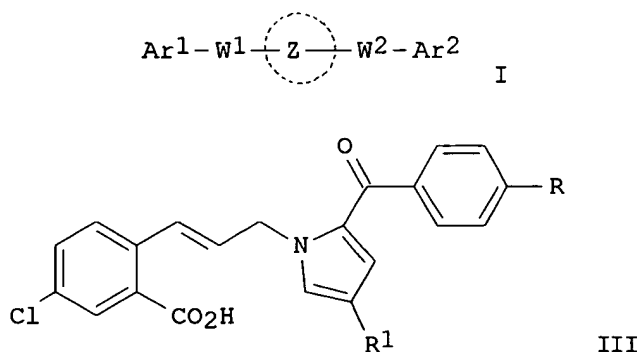
INVENTOR(S): Tokunaga, Teruhisa; Hume, William Ewan; Kitoh, Makoto;

Searcher : Shears 571-272-2528

10/088814

PATENT ASSIGNEE(S): Nagata, Ryu
 SOURCE: Sumitomo Pharmaceuticals Co., Ltd., Japan
 PCT Int. Appl., 215 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002010131	A1	20020207	WO 2001-JP6495	20010727
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001075794	A5	20020213	AU 2001-75794	20010727
CA 2416946	AA	20030122	CA 2001-2416946	20010727
EP 1310485	A1	20030514	EP 2001-953325	20010727
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003181496	A1	20030925	US 2003-352067	20030128
US 6759429	B2	20040706		
US 2004209939	A1	20041021	US 2004-840746	20040507
PRIORITY APPLN. INFO.:			JP 2000-229423	A 20000728
			WO 2001-JP6495	W 20010727
			US 2003-352067	A3 20030128
OTHER SOURCE(S):			MARPAT 136:167389	
GI				



AB The title compds. represented by the following formula (I) or pharmaceutically acceptable salts of these [wherein ring Z represents an optionally substituted pyrrole, indole, thiophene, pyrazole, benzene, imidazole, or isothiazole; W2 represents CO, SO2, CONR (R = H, alkyl), optionally substituted C1-4 alkylene or C2-4 alkenylene; Ar2 represents

optionally substituted aryl or heteroaryl; and W1 and Ar1 mean the following: (1) W1 represents optionally substituted C1-4 alkylene or C2-4 alkenylene, Ar1 represents bicyclic heteroaryl having one to four N atoms or (2) W1 represents optionally substituted C2-5 alkylene, C2-5 alkenylene, C2-5 alkynylene, or -Y-W3 (wherein Y = O or cycloalkanediyl; W3 = optionally substituted C1-5 alkylene, C2-5 alkenylene, or C2-5 alkynylene), Ar represents optionally substituted aryl or monocyclic heteroaryl substituted at ortho or meta position by CO₂H, alkoxy carbonyl, optionally alkyl-substituted carbamoyl, cyclic aminocarbonyl, alkylsulfonyl carbonyl, arylsulfonyl carbonyl, alkylsulfonyl, etc.] or prodrugs or pharmacol. acceptable salts thereof are prepared. These compds. are useful as fibroid inhibitors for organs or tissues. Thus, bromination of 3-(4-chloro-2-methoxycarbonylphenyl)-2-propenol (preparation given) by N-bromosuccinimide and PPh₃ in CH₂Cl₂ at 0° for 10 min gave 3-(4-chloro-2-methoxycarbonylphenyl)-2-propenyl bromide (II). A THF

solution

of 2-(4-methylbenzoyl)pyrrole was added dropwise to a suspension of NaH in THF and the resulting solution was slowly added dropwise to a THF solution of II

at 55° and stirred for 2 h to give 2-[3-[2-(4-methylbenzoyl)-1-pyrrolyl]-1-propen-1-yl]-5-chlorobenzoic acid Me ester which was saponified with aqueous NaOH in methanol and acidified with aqueous HCl to give III (R

= Me,

R1 = H). In a kidney fibroid model using a rat Thy-1 nephritis model, administration of III.Na (R = Me, R1 = H) at 15 mg/kg and Thy-1 (one of surface antigens of thymocyte) to rats lowered the level of hydroxyproline (fibroid index) in kidney compared to the control group administered only with Thy-1. III.Na (R = 2-morpholinoethoxy, R1 = Me) at 3 μM in vitro inhibited the TGF-β-induced production of proteoglycan in MRK-49F rat fibroblast cells by 99%.

IT **397323-98-7P**, 8-Cyano-2-[[2-(4-methylbenzoyl)pyrrol-1-yl]methyl]quinoxaline **397324-06-0P**, 5-Cyano-2-[[2-(4-methylbenzoyl)pyrrol-1-yl]methyl]quinoxaline **397324-14-0P**, 6-Cyano-2-[[2-(4-methylbenzoyl)pyrrol-1-yl]methyl]quinoxaline **397324-20-8P**, 7-Cyano-2-[[2-(4-methylbenzoyl)pyrrol-1-yl]methyl]quinoxaline **397325-01-8P**, 2-[[2-(4-Hydroxybenzoyl)pyrrol-1-yl]methyl]quinoxaline **397325-03-0P**, 2-[[2-(4-((Ethoxycarbonyl)methoxy)benzoyl)pyrrol-1-yl]methyl]quinoxaline
 RL: **PAC (Pharmacological activity); RCT (Reactant);**
 SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent); USES**
 (Uses)

(preparation of pyrrole, indole, thiophene, pyrazole, imidazole, and isothiazole derivs. as inhibitors of transforming growth factor-β and fibroid inhibitors for organs or tissues)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 36 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 01 Feb 2002

ACCESSION NUMBER: 2002:90040 CAPLUS

DOCUMENT NUMBER: 136:135022

TITLE: Preparation of heteroaryl-β-alanine derivatives as antiinflammatory agents and α4 integrin inhibitors

INVENTOR(S): Konradi, Andrei W.; Pleiss, Michael A.; Thorsett,

Eugene D.; Ashwell, Susan; Welmaker, Gregory S.; Kreft, Anthony; Sarantakis, Dimitrios; Dressen, Darren B.; Grant, Francine S.; Semko, Christopher; Xu, Ying-Zi

PATENT ASSIGNEE(S): Elan Pharmaceuticals, Inc., USA; American Home Products Corporation

SOURCE: PCT Int. Appl., 141 pp.
CODEN: PIXXD2

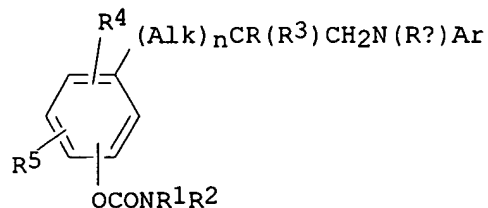
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008222	A2	20020131	WO 2001-US23096	20010720
WO 2002008222	A3	20020613		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002086882	A1	20020704	US 2001-910431	20010719
PRIORITY APPLN. INFO.:			US 2000-220128P	P 20000721
OTHER SOURCE(S):			MARPAT 136:135022	
GI				



AB Disclosed are a series of heteroaryl- β -alanine derivs. I wherein R is a carboxylic acid; R1 and R2 are independently selected from the group consisting of hydrogen, alkyl, substituted alkyl, alkenyl, substituted alkenyl, cycloalkyl, substituted cycloalkyl, or R1 and R2, together with the nitrogen atom to which they are attached, are joined to form an optionally substituted heterocyclic ring provided that said substituted alkyl, substituted alkenyl and substituted cycloalkyl do not carry an aryl, substituted aryl, heteroaryl or substituted heteroaryl group; Ra and R3 are independently a hydrogen or a Me group; R4 and R5 are independently selected from the group consisting of heteroatom group; n is zero or an integer 1; Alk is a straight or branched alkylene chain; Ar is an optionally substituted aromatic or heteroarom. group, as well as their

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pharmaceutical use as $\alpha 4\beta 7$ Integrin inhibitors for the treatment of inflammatory diseases. Thus, 3-[4-(3,5-dichloropyrid-4-ylcarboxamido)phenyl]-2-(3-chlorophenylamino)propanoic acid was prepared as $\alpha 4$ Integrin inhibitor. The preferred compds. of the invention generally have IC50 values in the $\alpha 4\beta 1$ and $\alpha a\beta 7$ assays of 1 μ M and below. In the other assays featuring α integrins of other subgroups the same compds. had IC50 values of 50 μ M and above thus demonstrating the potency and selectivity of their action against $\alpha 4$ integrins. Title compds. were prepared for treating an inflammatory condition in a mammalian patient which condition is mediated by Very Late Antigen 4 (VLA-4). Inflammatory condition is selected from the group consisting of asthma, Alzheimer's disease, atherosclerosis, AIDS dementia, diabetes, inflammatory bowel disease, multiple sclerosis, rheumatoid arthritis, tissue transplantation, tumor metastasis, meningitis, encephalitis, stroke, nephritis, retinitis, atopic dermatitis, psoriasis, myocardial ischemia and acute leukocyte-mediated lung injury.

IT 263275-09-8P 263275-11-2P

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of heteroaryl- β -alanine derivs. as antiinflammatory agents and $\alpha 4$ integrin inhibitors)

L22 ANSWER 37 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 01 Feb 2002

ACCESSION NUMBER: 2002:90026 CAPLUS

DOCUMENT NUMBER: 136:135019

TITLE: Preparation of 3-amino-2-(4-aminocarbonyloxy)phenyl-propionic acid derivatives as antiinflammatory agents and $\alpha 4$ Integrin inhibitors

INVENTOR(S): Konradi, Andrei W.; Pleiss, Michael A.; Thorsett, Eugene D.; Ashwell, Susan; Welmaker, Gregory S.; Kreft, Anthony; Sarantakis, Dimitrios; Dressen, Darren B.; Grant, Francine S.; Xu, Ying-Zi

PATENT ASSIGNEE(S): Elan Pharmaceuticals, Inc., USA; American Home Products Corporation

SOURCE: PCT Int. Appl., 137 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

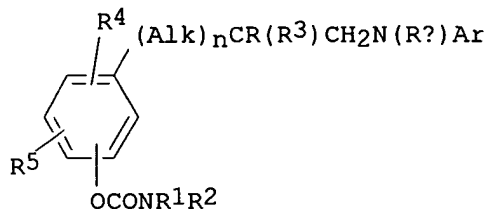
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008206	A1	20020131	WO 2001-US23073	20010720
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

Searcher : Shears 571-272-2528

10/088814

US 2002055509	A1	20020509	US 2001-910685	20010720
US 6689781	B2	20040210		
US 2004127486	A1	20040701	US 2003-735499	20031212
PRIORITY APPLN. INFO.:			US 2000-220134P	P 20000721
			US 2001-910685	A3 20010720
OTHER SOURCE(S):		MARPAT 136:135019		
GI				



AB 3-Amino-2-(4-aminocarboxyloxy)phenyl-propionic acid derivs. I wherein R is a carboxylic acid; R1 and R2 are independently selected from the group consisting of hydrogen, alkyl, substituted alkyl, alkenyl, substituted alkenyl, cycloalkyl, substituted cycloalkyl, or R1 and R2, together with the nitrogen atom to which they are attached, are joined to form an optionally substituted heterocyclic ring provided that said substituted alkyl, substituted alkenyl and substituted cycloalkyl do not carry an aryl, substituted aryl, heteroaryl or substituted heteroaryl group; Ra and R3 are independently a hydrogen or a Me group; R4 and R5 are independently selected from the group consisting of heteroatom group; n is zero or an integer 1; Alk is a straight or branched alkylene chain; Ar is an optionally substituted aromatic or heteroarom. group, as well as their pharmaceutical use as $\alpha 4\beta 7$ Integrin inhibitors for the treatment of inflammatory diseases. Thus, 3-[4-(3,5-dichloropyrid-4-ylcarboxamido)phenyl]-2-(3-chlorophenylamino)propanoic acid was prepared as $\alpha 4$ Integrin inhibitor. The preferred compds. of the invention generally have IC50 values in the $\alpha 4\beta 1$ and $\alpha 4\beta 7$ assays of 1 μ M and below. In the other assays featuring α integrins of other subgroups the same compds. had IC50 values of 50 μ M and above thus demonstrating the potency and selectivity of their action against $\alpha 4$ integrins. Title compds. were prepared for treating an inflammatory condition in a mammalian patient which condition is mediated by Very Late Antigen 4 (VLA-4). Inflammatory condition is selected from the group consisting of asthma, Alzheimer's disease, atherosclerosis, AIDS dementia, diabetes, inflammatory bowel disease, multiple sclerosis, rheumatoid arthritis, tissue transplantation, tumor metastasis, meningitis, encephalitis, stroke, nephritis, retinitis, atopic dermatitis, psoriasis, myocardial ischemia and acute leukocyte-mediated lung injury.

IT 263275-09-8P 263275-11-2P

RL: IMF (Industrial manufacture); PAC (Pharmacological activity)
; RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic
use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or
reagent); USES (Uses)

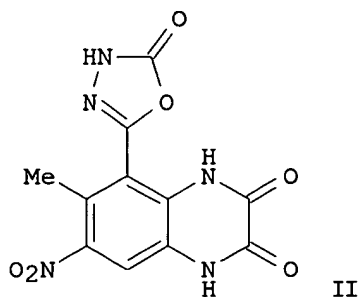
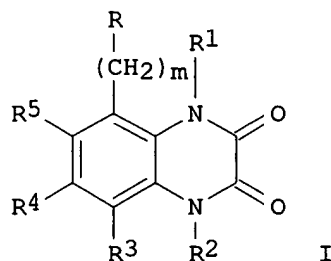
(preparation of aminoaminocarbonyloxyphenylpropionic acid derivs. as a integrin inhibitors)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Searcher : Shears 571-272-2528

L22 ANSWER 38 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
 ED Entered STN: 24 Jan 2002
 ACCESSION NUMBER: 2002:66864 CAPLUS
 DOCUMENT NUMBER: 136:118473
 TITLE: Preparation of conformationally semi-constrained
 quinoxaline-2,3-diones as neuroprotective agents
 INVENTOR(S): Kornberg, Brian Edward; Nikam, Sham Shridhar;
 Rafferty, Michael Francis
 PATENT ASSIGNEE(S): Warner-Lambert Company, USA
 SOURCE: U.S., 27 pp., Cont.-in-part of U.S. Ser. No. 25,295,
 now abandoned.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6340758	B1	20020122	US 1998-199627	19981125
US 2002065415	A1	20020530	US 2001-971237	20011004
US 6455698	B2	20020924		
PRIORITY APPLN. INFO.:			US 1997-46626P	P 19970516
			US 1998-25295	B2 19980213
			US 1998-199627	A3 19981125
OTHER SOURCE(S):	MARPAT 136:118473			
GI				



AB Title compds. I [wherein R = (un)substituted azacyclo, substituted carboxamido, piperazinocarbonyl, or diazepanylcabonyl; R2 = H; R3 = H; R4 = independently H, (cyclo)alkyl, alkenyl, halo(alkyl), NO2, CN, SO2CF3, CH2SO2R7, (CH2)mCO2R7, (CH2)mCONR7R8, (CH2)mSO2NR8R9, or NHCOR7; R7, R8, and R9 = independently H, (cyclo)alkyl, haloalkyl, or (CH2)mR11; R11 = alkyl, alkoxy, OH, or NH2; m = 0-4; or pharmaceutically acceptable salts thereof], as well as 2,3-dimethoxyquinoxaline-5-carboxamides, were prepared as neuroprotective agents. For example, cycloaddn. of di-Me oxalate with 2,3-diamino-6-methylbenzoic acid Me ester (6-step preparation from anthranilic acid given) afforded 6-methyl-2,3-dioxo-1,2,3,4-tetrahydroquinoxaline-5-carboxylic acid Me ester (69%). Nitration (97%), followed by hydrazide formation (80%) and cycloaddn. with phosgene (50%), afforded

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6-methyl-7-nitro-5-(5-oxo-4,5-dihydro-[1,3,4]oxadiazol-2-yl)-1,4-dihydroquinoxaline-2,3-dione (II). The latter exhibited strong excitatory amino acid antagonizing properties at the AMPA binding site on the AMPA glutamate receptor.

IT 258508-93-9P, [(2,3-Dimethoxy-6-methyl-7-nitroquinoxaline-5-carbonyl)amino]acetic acid tert-butyl ester

RL: PAC (Pharmacological activity); RCT (Reactant);

SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(neuroprotective agent; preparation of conformationally semi-constrained quinoxalinediones and dimethoxyquinoxalinecarboxamides as neuroprotective agents)

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 39 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN

ED Entered STN: 13 May 2001

ACCESSION NUMBER: 2001:340055 CAPLUS

DOCUMENT NUMBER: 136:102343

TITLE: Synthesis and anticancer activity of some novel 2-(quinoxalin-2-yl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidine derivatives

AUTHOR(S): Ismail, M. M. F.; Zahran, Medhat A.; El-Gaby, M. S. A.; Ammar, Y. A.

CORPORATE SOURCE: Chemistry Department, Faculty of Pharmacy (Girl's), Al-Azhar University, Nasr City, Egypt

SOURCE: Al-Azhar Bulletin of Science (1999), 10(1), 41-50
CODEN: ABSCE7; ISSN: 1110-2535

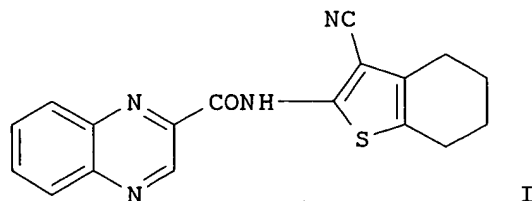
PUBLISHER: Al-Azhar University, Faculty of Science

DOCUMENT TYPE: Journal

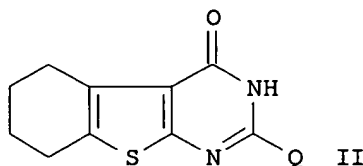
LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:102343

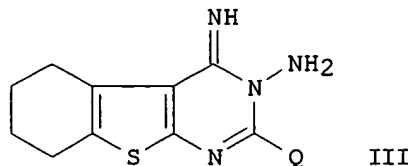
GI



I



II



III

AB 2-Carboxamide derivative I was obtained by a fusion reaction and refluxing of

Searcher : Shears 571-272-2528

10/088814

I in acetic anhydride afforded thieno[2,3-d]pyrimidine II (Q = 2-quinoxaliny). Cyclization of the intermediate I with hydrazine hydrate in refluxing butanol furnished a thieno[2,3-d]pyrimidine derivative III (Q = 2-quinoxaliny). Reaction of III with aromatic aldehydes led to the formation of Schiff's bases. A thiourea derivative was obtained by refluxing of III with Ph isothiocyanate in pyridine. Preliminary pharmacol. screening revealed that some of the new compds. exhibited anticancer activity.

IT 389085-71-6P 389085-74-9P 389085-81-8P

RL: PAC (Pharmacological activity); RCT (Reactant);

SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation);

RACT (Reactant or reagent)

(preparation and anticancer activity of (quinoxaliny)tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidine derivs.)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

E1 THROUGH E131 ASSIGNED

FILE 'REGISTRY' ENTERED AT 09:54:59 ON 07 FEB 2005

L23 131 SEA FILE=REGISTRY ABB=ON PLU=ON (263275-09-8/BI OR 263275-11-2/BI OR 612847-29-7/BI OR 14121-55-2/BI OR 168835-90-3/BI OR 1865-11-8/BI OR 187479-25-0/BI OR 187479-26-1/BI OR 215238-12-3/BI OR 217093-53-3/BI OR 223929-23-5/BI OR 258508-93-9/BI OR 278186-19-9/BI OR 313654-02-3/BI OR 313656-86-9/BI OR 313656-92-7/BI OR 389085-71-6/BI OR 389085-74-9/BI OR 389085-81-8/BI OR 397323-98-7/BI OR 397324-06-0/BI OR 397324-14-0/BI OR 397324-20-8/BI OR 397325-01-8/BI OR 397325-03-0/BI OR 444807-95-8/BI OR 459836-02-3/BI OR 459836-07-8/BI OR 459836-08-9/BI OR 459836-09-0/BI OR 459836-14-7/BI OR 459836-15-8/BI OR 459836-22-7/BI OR 462119-65-9/BI OR 462119-66-0/BI OR 462119-67-1/BI OR 462119-68-2/BI OR 462119-69-3/BI OR 474777-33-8/BI OR 476374-02-4/BI OR 476374-03-5/BI OR 476374-04-6/BI OR 476374-05-7/BI OR 476374-06-8/BI OR 476374-07-9/BI OR 476374-08-0/BI OR 476374-09-1/BI OR 476374-10-4/BI OR 476374-11-5/BI OR 476374-12-6/BI OR 476374-13-7/BI OR 476374-14-8/BI OR 476374-15-9/BI OR 476374-16-0/BI OR 476374-17-1/BI OR 476374-18-2/BI OR 476374-27-3/BI OR 495407-42-6/BI OR 495407-43-7/BI OR 495407-45-9/BI OR 570405-07-1/BI OR 59803-98-4/BI OR 612847-30-0/BI OR 612847-31-1/BI OR 612847-32-2/BI OR 612848-47-2/BI OR 612848-75-6/BI OR 612848-76-7/BI OR 623583-65-3/BI OR 623934-58-7/BI OR 623934-59-8/BI OR 642478-38-4/BI OR 643069-13-0/BI OR 643069-72-1/BI OR 643069-97-0/BI OR 643070-09-1/BI OR 643070-52-4/BI OR 643070-54-6/BI OR 659729-63-2/BI OR 659729-66-5/BI OR 659729-73-4/BI OR 663191-50-2/BI OR 681235-15-4/BI OR 681235-17-6/BI OR 683273-27-0/BI OR 692246-95-0/BI OR 694528-79-5/BI OR 694528-80-8/BI OR 694528-84-2/BI OR 694528-95-5/BI OR 694528-97-7/BI OR 694529-00-5/BI OR 694529-55-0/BI OR 694530-66-0/BI OR 694531-07-2/BI OR 694531-12-9/BI OR 694531-13-0/BI OR 694531-15-2/BI OR 694531-18-5/BI OR 694531-

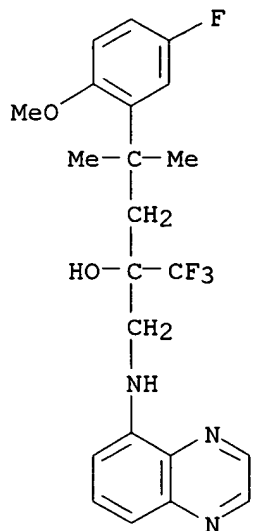
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STrs displayed
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1-5, 7, 25, 27, 29, 36, 37, 39, 44-46, 48, 49, 52, 55, 58, 59, 61, 62, 65, 69, 70, 73, 91, 92, 97, 104, 105, 107, 111, 114, 116-124, 126-131 ide can

Searcher : Shears 571-272-2528

10/088814

L23 ANSWER 1 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 825653-48-3 REGISTRY
CN INDEX NAME NOT YET ASSIGNED
MF C22 H23 F4 N3 O2
SR CA
LC STN Files: CAPLUS
DT.CA Caplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)

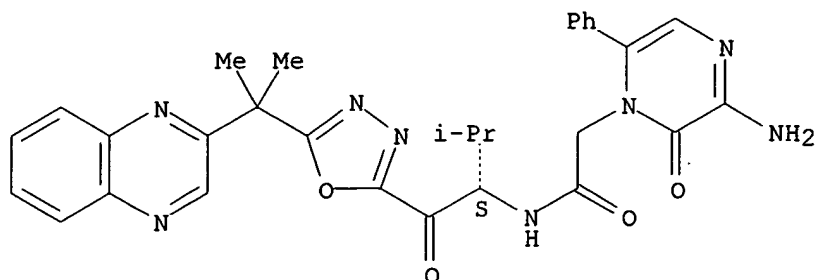


1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L23 ANSWER 2 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 757970-18-6 REGISTRY
CN 1(2H)-Pyrazineacetamide, 3-amino-N-[(1S)-2-methyl-1-[[5-[1-methyl-1-(2-quinoxaliny)ethyl]-1,3,4-oxadiazol-2-yl]carbonyl]propyl]-2-oxo-6-phenyl-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H30 N8 O4
SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)

Absolute stereochemistry.

10/088814



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:277626

L23 ANSWER 3 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 717103-60-1 REGISTRY

CN Methanone, [2-[[(2,3-dimethoxy-6-quinoxaliny)l)methyl]amino]-5-(2-propynyloxy)phenyl][4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN [2-[[(2,3-Dimethoxyquinoxalin-6-yl)methyl]amino]-5-((prop-2-ynyl)oxy)phenyl][4-isopropylphenyl)methanone

FS 3D CONCORD

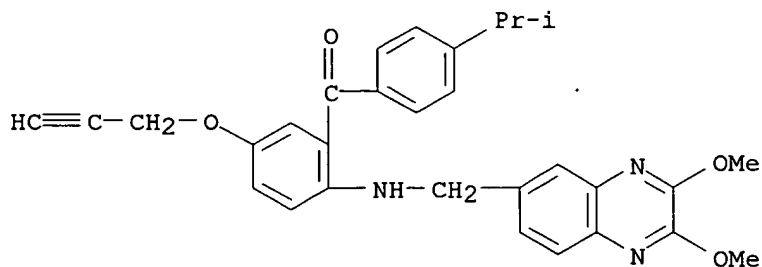
MF C30 H29 N3 O4

SR CA

LC STN Files: CA, CAPLUS

DT.CA Caplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

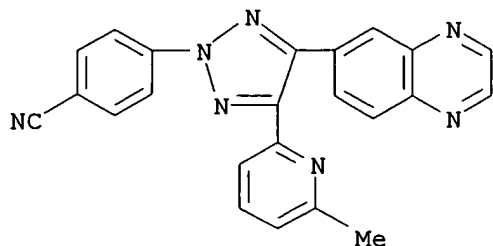
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:89103

Searcher : Shears 571-272-2528

10/088814

L23 ANSWER 4 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 710947-10-7 REGISTRY
CN Benzonitrile, 4-[4-(6-methyl-2-pyridinyl)-5-(6-quinoxaliny)-2H-1,2,3-
triazol-2-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H15 N7
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation);
RACT (Reactant or reagent)

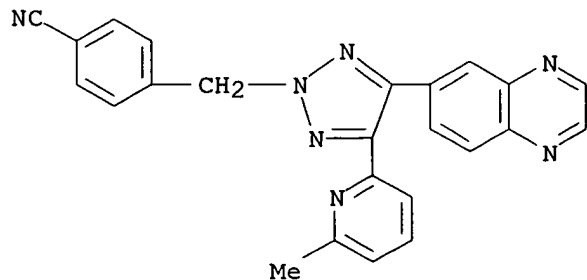


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:71490

L23 ANSWER 5 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 710946-99-9 REGISTRY
CN Benzonitrile, 4-[[4-(6-methyl-2-pyridinyl)-5-(6-quinoxaliny)-2H-1,2,3-
triazol-2-yl]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H17 N7
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation);
RACT (Reactant or reagent)



Searcher : Shears 571-272-2528

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:71490

L23 ANSWER 7 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 709638-58-4 REGISTRY

CN L-Glutamic acid, N-[[4-[[3-[[[(1S)-4-ethoxy-1-(ethoxycarbonyl)-4-oxobutyl]amino]carbonyl]-6-(trifluoromethyl)-2-quinoxalinyloxy]phenyl]acetyl]-, diethyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C36 H41 F3 N4 O11

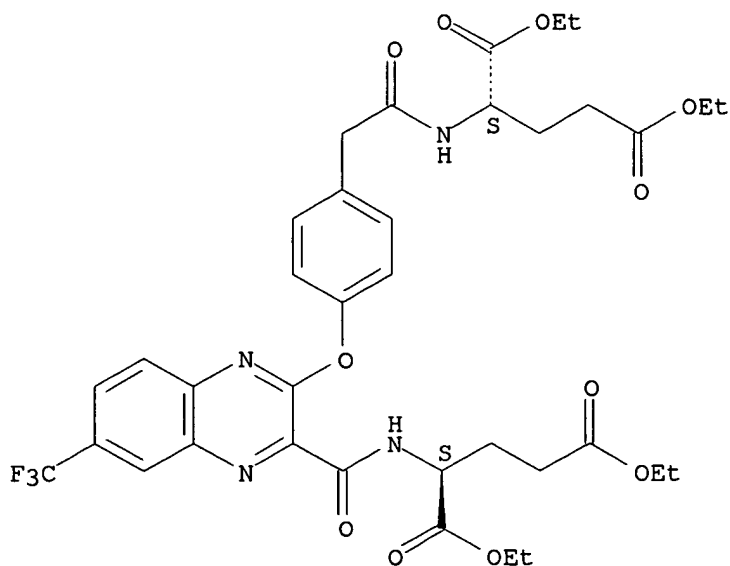
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation);
PRP (Properties); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry.



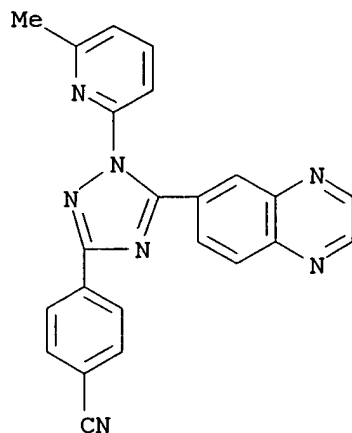
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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:64522

10/088814

L23 ANSWER 25 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 701979-19-3 REGISTRY
CN Benzonitrile, 4-[1-(6-methyl-2-pyridinyl)-5-(6-quinoxaliny)-1H-1,2,4-
triazol-3-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H15 N7
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation);
PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

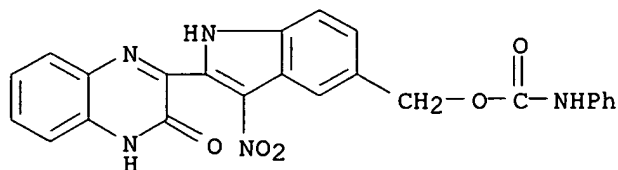
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:33319

L23 ANSWER 27 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 694532-22-4 REGISTRY
CN 2(1H)-Quinoxalinone, 3-[3-nitro-5-[[[(phenylamino)carbonyl]oxy]methyl]-1H-
indol-2-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H17 N5 O5
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)

Searcher : Shears 571-272-2528

10/088814

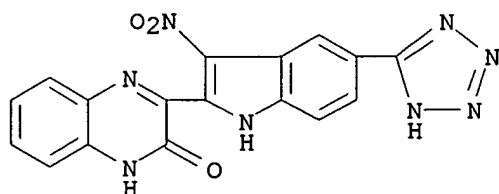


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:7139

L23 ANSWER 29 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 694531-42-5 REGISTRY
CN 2(1H)-Quinoxalinone, 3-[3-nitro-5-(1H-tetrazol-5-yl)-1H-indol-2-yl]- (9CI)
(CA INDEX NAME)
FS 3D CONCORD
MF C17 H10 N8 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

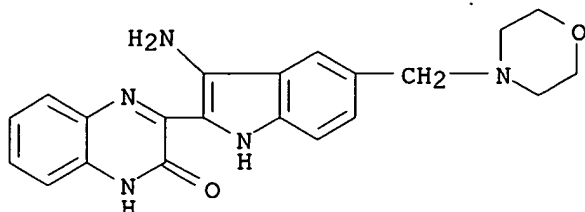
REFERENCE 1: 141:7139

L23 ANSWER 36 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 694530-66-0 REGISTRY
CN 2(1H)-Quinoxalinone, 3-[3-amino-5-(4-morpholinylmethyl)-1H-indol-2-yl]-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H21 N5 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent

Searcher : Shears 571-272-2528

10/088814

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

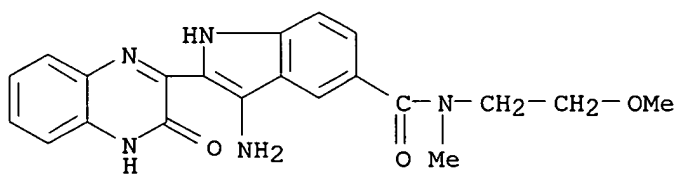


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:7139

L23 ANSWER 37 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 694529-55-0 REGISTRY
CN 1H-Indole-5-carboxamide, 3-amino-2-(3,4-dihydro-3-oxo-2-quinoxaliny)-N-(2-methoxyethyl)-N-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H21 N5 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA Caplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

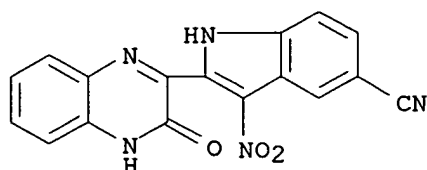
REFERENCE 1: 141:7139

L23 ANSWER 39 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 694528-97-7 REGISTRY
CN 1H-Indole-5-carbonitrile, 2-(3,4-dihydro-3-oxo-2-quinoxaliny)-3-nitro- (9CI) (CA INDEX NAME)
FS 3D CONCORD

Searcher : Shears 571-272-2528

10/088814

MF C17 H9 N5 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA Caplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

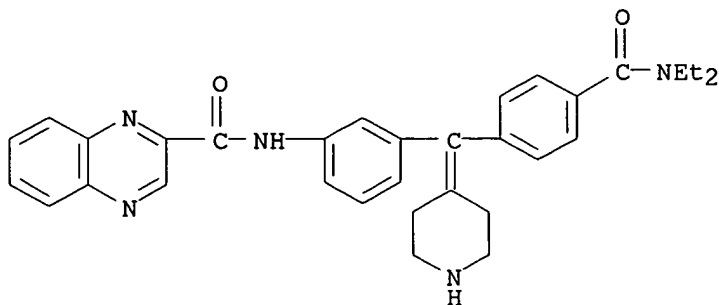
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:7139

L23 ANSWER 44 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 692246-95-0 REGISTRY
CN 2-Quinoxalinecarboxamide, N-[3-[[4-[(diethylamino)carbonyl]phenyl]-4-piperidinylidenemethyl]phenyl]-, trifluoroacetate (10:11) (9CI) (CA INDEX NAME)
MF C32 H33 N5 O2 . 11/10 C2 H F3 O2
SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)

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CRN 692246-93-8
CMF C32 H33 N5 O2



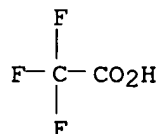
Searcher : Shears 571-272-2528

10/088814

CM 2

CRN 76-05-1

CMF C2 H F3 O2



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:423590

L23 ANSWER 45 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 683273-27-0 REGISTRY

CN Benzamide, 4-[(1E)-3-[[2-[[2,4-dichloro-3-[(2-methyl-5-quinoxalinyloxy)methyl]phenyl]methylamino]-2-oxoethyl]amino]-3-oxo-1-propenyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C30 H27 Cl2 N5 O4 . Cl H

SR CA

LC STN Files: CA, CAPLUS

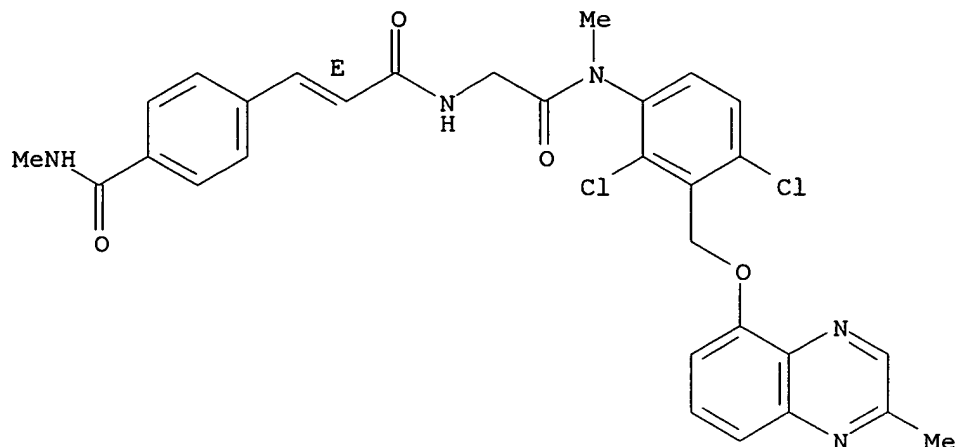
DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

CRN (215238-13-4)

Double bond geometry as shown.

10/088814



● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:368093

L23 ANSWER 46 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 681235-17-6 REGISTRY

CN Hydrazinecarbothioamide, N-[4-[(2-quinoxalinylamino)sulfonyl]phenyl]-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

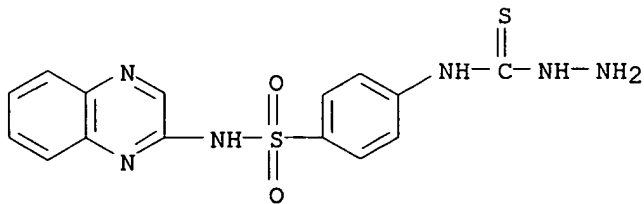
MF C15 H14 N6 O2 S2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation);
RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

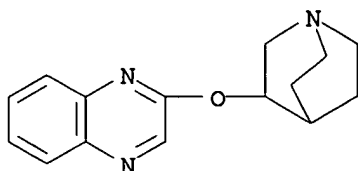
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Searcher : Shears 571-272-2528

10/088814

REFERENCE 1: 140:357296

L23 ANSWER 48 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **663191-50-2** REGISTRY
CN 1-Azabicyclo[2.2.2]octane, 3-(2-quinoxalinyloxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H17 N3 O
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA Caplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)

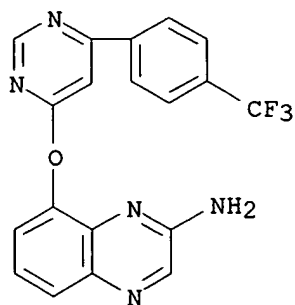


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:199493

L23 ANSWER 49 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **659729-73-4** REGISTRY
CN 2-Quinoxalinamine, 8-[[6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]oxy]-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H12 F3 N5 O
SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)



Searcher : Shears 571-272-2528

10/088814

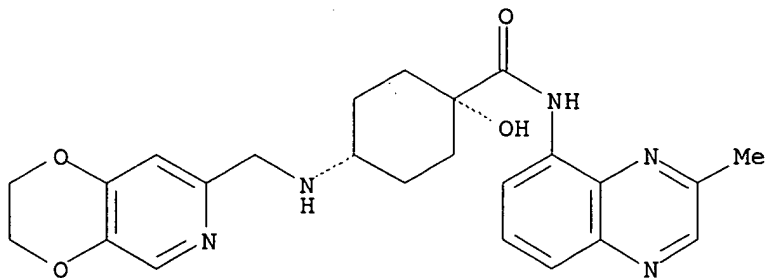
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1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:181462

L23 ANSWER 52 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 643070-54-6 REGISTRY
CN Cyclohexanecarboxamide, 4-[[(2,3-dihydro-1,4-dioxino[2,3-c]pyridin-7-yl)methyl]amino]-1-hydroxy-N-(3-methyl-5-quinoxaliny)-, cis- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H27 N5 O4
CI COM
SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:94053

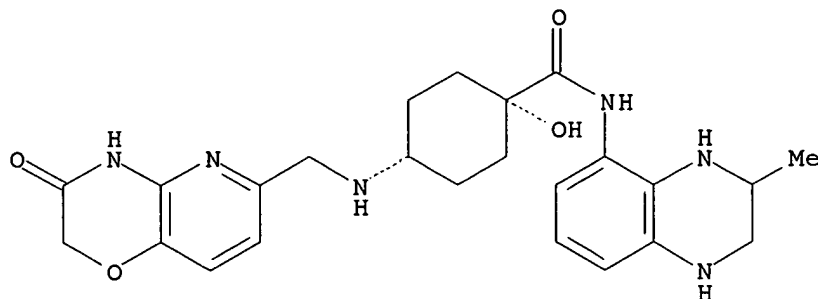
L23 ANSWER 55 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 643069-97-0 REGISTRY
CN Cyclohexanecarboxamide, 4-[[(3,4-dihydro-3-oxo-2H-pyrido[3,2-b]-1,4-oxazin-6-yl)methyl]amino]-1-hydroxy-N-(1,2,3,4-tetrahydro-3-methyl-5-quinoxaliny)-, cis- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H30 N6 O4
CI COM
SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Patent

Searcher : Shears 571-272-2528

10/088814

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:94053

L23 ANSWER 58 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 642478-38-4 REGISTRY

CN 5-Quinoxalinemethanol, α -[[4-[(2,3-dihydro-1,4-dioxino[2,3-c]pyridin-7-yl)methyl]amino]-1-piperidinyl]methyl]-3-methoxy- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C24 H29 N5 O4

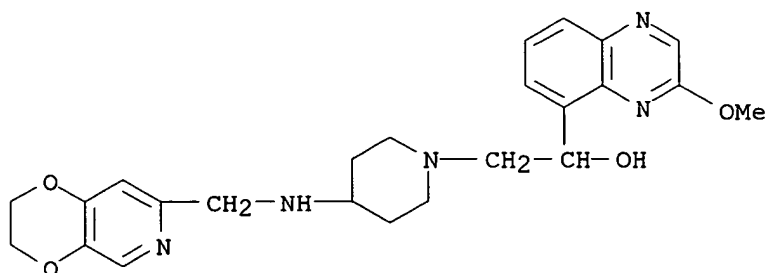
CI COM

SR CA

LC STN Files: CA, CAPLUS

DT.CA Caplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

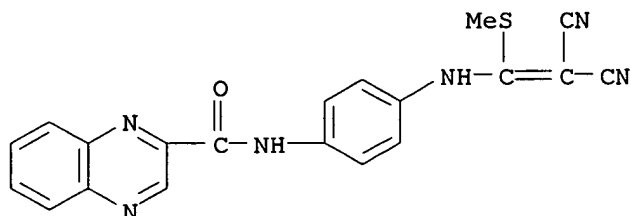
Searcher : Shears 571-272-2528

10/088814

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:94052

L23 ANSWER 59 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **623934-59-8** REGISTRY
CN 2-Quinoxalinecarboxamide, N-[4-[[2,2-dicyano-1-(methylthio)ethenyl]amino]phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H14 N6 O S
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

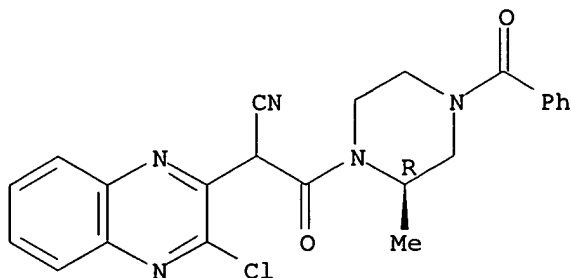
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:381448

L23 ANSWER 61 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **623583-65-3** REGISTRY
CN Piperazine, 4-benzoyl-1-[(3-chloro-2-quinoxaliny)cyanoacetyl]-2-methyl-, (2R)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H20 Cl N5 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA Caplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry.

10/088814

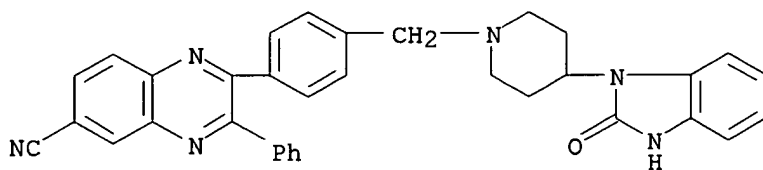


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:381510

L23 ANSWER 62 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **612848-76-7** REGISTRY
CN 6-Quinoxalinecarbonitrile, 2-[4-[[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)-1-piperidiny]methyl]phenyl]-3-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C34 H28 N6 O
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA Caplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:350754

REFERENCE 2: 139:323527

L23 ANSWER 65 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **612847-32-2** REGISTRY
CN 6-Quinoxalinecarboxylic acid, 2-[4-[[4-(2,3-dihydro-2-oxo-1H-benzimidazol-

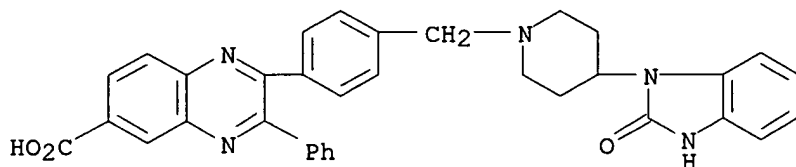
Searcher : Shears 571-272-2528

10/088814

1-yl)-1-piperidiny]methyl]phenyl]-3-phenyl-, trifluoroacetate (9CI) (CA
INDEX NAME)
MF C34 H29 N5 O3 . x C2 H F3 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)

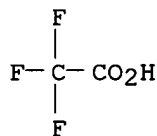
CM 1

CRN 612847-31-1
CMF C34 H29 N5 O3



CM 2

CRN 76-05-1
CMF C2 H F3 O2



3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:7131

REFERENCE 2: 139:350754

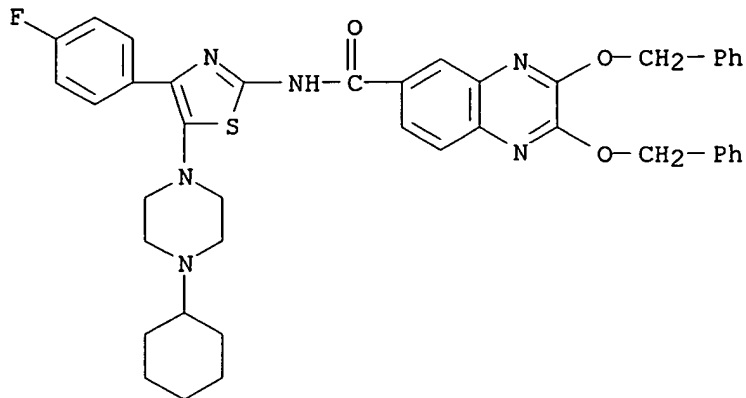
REFERENCE 3: 139:323527

L23 ANSWER 69 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 570405-07-1 REGISTRY
CN 6-Quinoxalinecarboxamide, N-[5-(4-cyclohexyl-1-piperazinyl)-4-(4-
fluorophenyl)-2-thiazolyl]-2,3-bis(phenylmethoxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C42 H41 F N6 O3 S
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT

Searcher : Shears 571-272-2528

10/088814

(Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:149652

L23 ANSWER 70 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN **495407-45-9** REGISTRY

CN Acetic acid, [3,4-dihydro-3-oxo-8-(phenylmethoxy)-2(1H)-quinoxalinyldene]-
, ethyl ester (9CI) (CA INDEX NAME)

OTHER NAMES:

CN Ethyl [8-(benzyloxy)-3-oxo-3,4-dihydroquinoxaline-2(1H)-ylidene]acetate

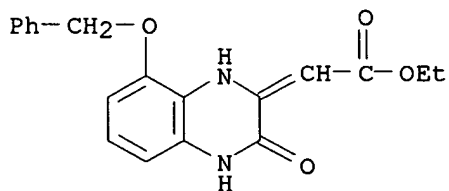
MF C19 H18 N2 O4

SR CA

LC STN Files: CA, CAPLUS

DT.CA Caplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

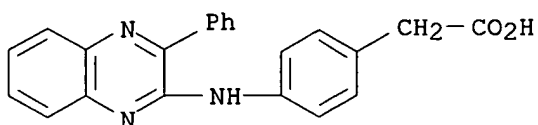
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Searcher : Shears 571-272-2528

10/088814

REFERENCE 1: 138:153554

L23 ANSWER 73 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **476374-27-3** REGISTRY
CN Benzeneacetic acid, 4-[(3-phenyl-2-quinoxaliny)amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H17 N3 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

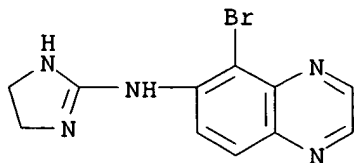
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:83

L23 ANSWER 91 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **474777-33-8** REGISTRY
CN 9,12-Octadecadienoic acid (9Z,12Z)-, compd. with 5-bromo-N-(4,5-dihydro-1H-imidazol-2-yl)-6-quinoxalinamine (1:1) (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C18 H32 O2 . C11 H10 Br N5
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
DT.CA Caplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

CM 1

CRN 59803-98-4
CMF C11 H10 Br N5



Searcher : Shears 571-272-2528

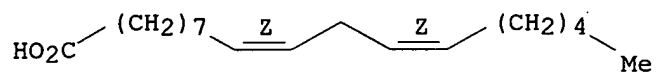
10/088814

CM 2

CRN 60-33-3

CMF C18 H32 O2

Double bond geometry as shown.



3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:226731

REFERENCE 2: 138:112477

REFERENCE 3: 137:358171

L23 ANSWER 92 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 462119-69-3 REGISTRY

CN 6-Quinoxalinecarboxamide, N-[3-[5-[[[(1R)-3-amino-1-(1-piperazinylcarbonyl)propyl]amino]carbonyl]-2-furanyl]propyl]-1,2,3,4-tetrahydro-2,3-dioxo- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C25 H31 N7 O6

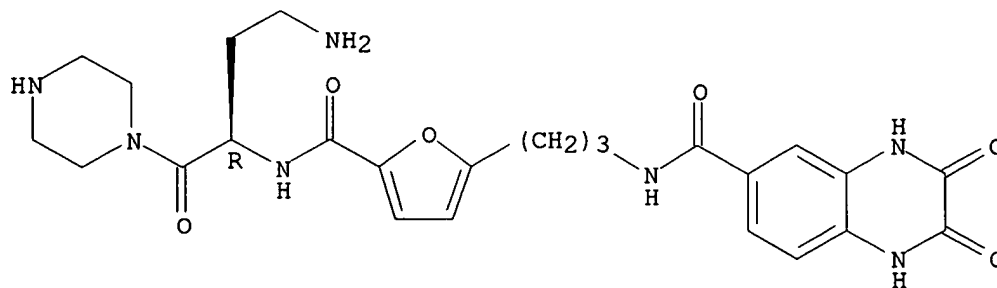
SR CA

LC STN Files: CA, CAPLUS, CASREACT

DT.CA Cplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

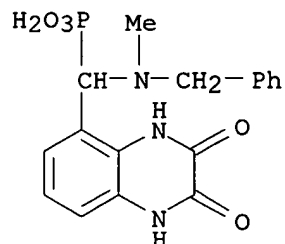
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:257239

Searcher : Shears 571-272-2528

10/088814

L23 ANSWER 97 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **459836-22-7** REGISTRY
CN Phosphonic acid, [[methyl(phenylmethyl)amino](1,2,3,4-tetrahydro-2,3-dioxo-5-quinoxaliny)methyl]- (9CI) (CA INDEX NAME)
MF C17 H18 N3 O5 P
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

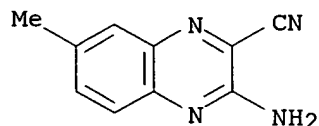


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:226178

L23 ANSWER 104 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **444807-95-8** REGISTRY
CN 2-Quinoxalinecarbonitrile, 3-amino-7-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H8 N4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Searcher : Shears 571-272-2528

10/088814

REFERENCE 1: 141:133557

REFERENCE 2: 137:134476

L23 ANSWER 105 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 397325-03-0 REGISTRY

CN Acetic acid, [4-[[1-(2-quinoxalinylmethyl)-1H-pyrrol-2-yl]carbonyl]phenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 2-[[2-(4-((Ethoxycarbonyl)methoxy)benzoyl)pyrrol-1-yl)methyl]quinoxaline

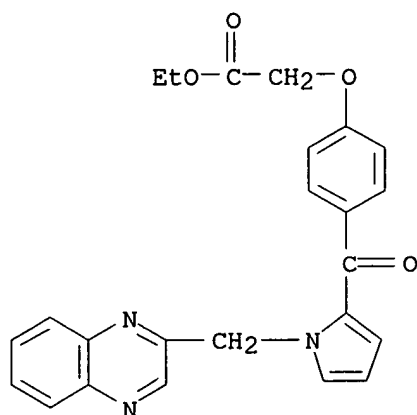
MF C24 H21 N3 O4

SR CA

LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

DT.CA Caplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:159972

REFERENCE 2: 136:167389

L23 ANSWER 107 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 397324-20-8 REGISTRY

CN 6-Quinoxalinecarbonitrile, 3-[[2-(4-methylbenzoyl)-1H-pyrrol-1-yl)methyl]- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 7-Cyano-2-[[2-(4-methylbenzoyl)pyrrol-1-yl)methyl]quinoxaline

FS 3D CONCORD

MF C22 H16 N4 O

SR CA

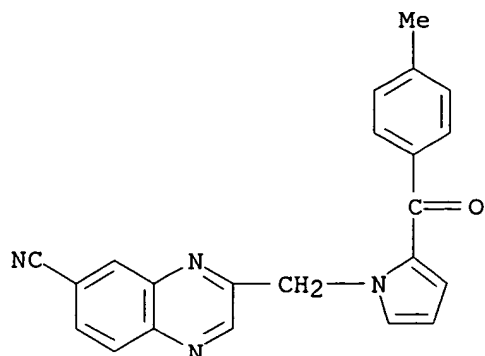
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

DT.CA Caplus document type: Patent

Searcher : Shears 571-272-2528

10/088814

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:159972

REFERENCE 2: 136:167389

L23 ANSWER 111 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 389085-81-8 REGISTRY

CN 2-Quinoxalinecarboxylic acid, 3-[[3-cyano-4,5,6,7-tetrahydrobenzo[b]thien-2-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

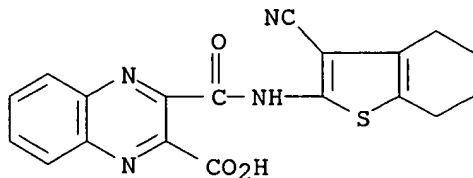
MF C19 H14 N4 O3 S

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Searcher : Shears 571-272-2528

10/088814

REFERENCE 1: 136:102343

L23 ANSWER 114 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN **313656-92-7** REGISTRY

CN Quinoxaline, 6,7-dichloro-2-(1-piperazinyl)-3-[2-(3-pyridinyloxy)ethoxy]-
(9CI) (CA INDEX NAME)

OTHER NAMES:

CN 2-[2-(3-Pyridinyloxy)ethoxy]-3-(1-piperazinyl)-6,7-dichloroquinoxaline

FS 3D CONCORD

MF C19 H19 Cl2 N5 O2

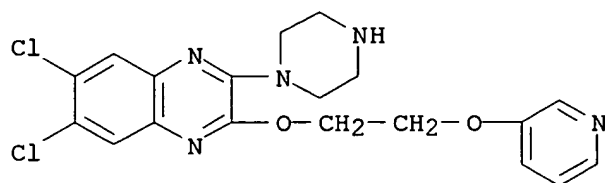
CI COM

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

DT.CA Caplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:294982

REFERENCE 2: 134:56689

L23 ANSWER 116 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN **313654-02-3** REGISTRY

CN Quinoxaline, 2-(2-phenoxyethoxy)-3-(1-piperazinyl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 2-(2-Phenoxyethoxy)-3-(1-piperazinyl)quinoxaline

FS 3D CONCORD

MF C20 H22 N4 O2

CI COM

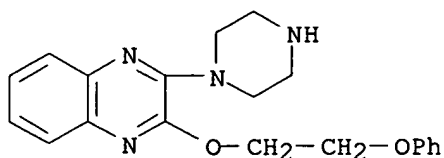
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

DT.CA Caplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)

10/088814



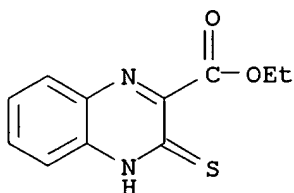
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:294982

REFERENCE 2: 134:56689

L23 ANSWER 117 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 278186-19-9 REGISTRY
CN 2-Quinoxalinecarboxylic acid, 3,4-dihydro-3-thioxo-, ethyl ester (9CI)
(CA INDEX NAME)
FS 3D CONCORD
MF C11 H10 N2 O2 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation);
RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:78924

REFERENCE 2: 136:263138

REFERENCE 3: 133:58781

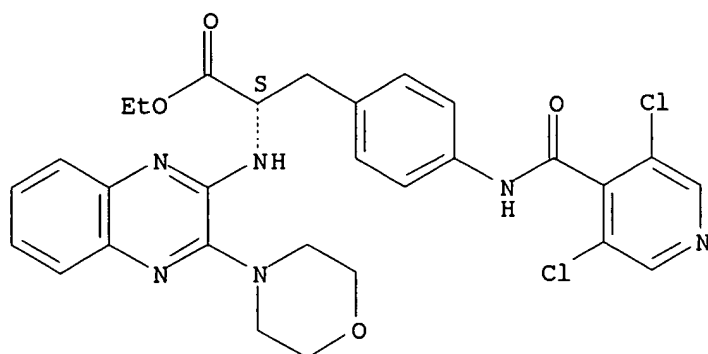
L23 ANSWER 118 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 263275-11-2 REGISTRY
CN L-Phenylalanine, 4-[[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[3-(4-

Searcher : Shears 571-272-2528

10/088814

morpholinyl)-2-quinoxalinyll]-, ethyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H28 Cl2 N6 O4
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
DT.CA Caplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:135022

REFERENCE 2: 136:135019

REFERENCE 3: 132:265501

L23 ANSWER 119 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 263275-09-8 REGISTRY

CN L-Phenylalanine, N-(3-chloro-2-quinoxalinyll)-4-[[3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C23 H16 Cl3 N5 O3

SR CA

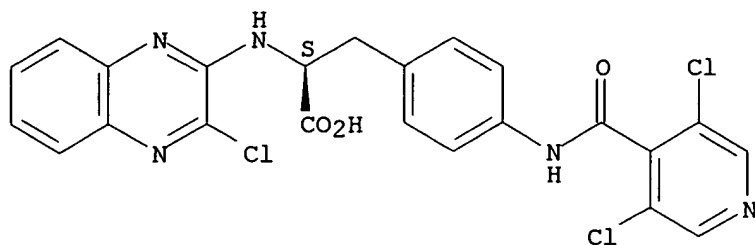
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

DT.CA Caplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)

Absolute stereochemistry.

10/088814



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:135022

REFERENCE 2: 136:135019

REFERENCE 3: 132:265501

L23 ANSWER 120 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 258508-93-9 REGISTRY

CN Glycine, N-[(2,3-dimethoxy-6-methyl-7-nitro-5-quininoxaliny)carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

OTHER NAMES:

CN [(2,3-Dimethoxy-6-methyl-7-nitroquininoxaline-5-carbonyl)amino]acetic acid tert-butyl ester

FS 3D CONCORD

MF C18 H22 N4 O7

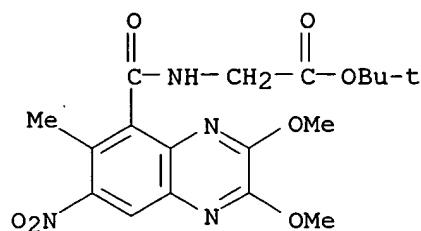
SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Searcher : Shears 571-272-2528

10/088814

REFERENCE 1: 136:118473

REFERENCE 2: 132:166212

L23 ANSWER 121 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN **223929-23-5** REGISTRY

CN 2(1H)-Quinoxalinone, 3-(phenylmethyl)-, hydrazone (9CI) (CA INDEX NAME)

OTHER NAMES:

CN (3-Benzylquinoxalin-2-yl)hydrazine

FS 3D CONCORD

MF C15 H14 N4

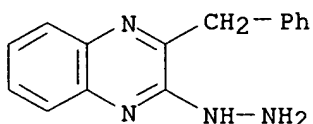
SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

DT.CA Cplus document type: Journal; Patent

RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation);
RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:314272

REFERENCE 2: 139:36744

REFERENCE 3: 132:237060

REFERENCE 4: 130:325156

L23 ANSWER 122 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN **217093-53-3** REGISTRY

CN 2-Azabicyclo[2.2.2]octan-3-one, 2-(6,7-dimethoxy-2-quinoxaliny)- (9CI)
(CA INDEX NAME)

FS 3D CONCORD

MF C17 H19 N3 O3

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL

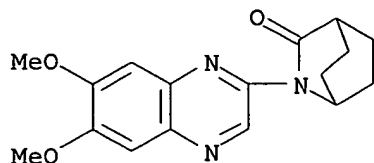
DT.CA Cplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation);
RACT (Reactant or reagent); USES (Uses)

Searcher : Shears 571-272-2528

10/088814



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:285655

REFERENCE 2: 134:131553

REFERENCE 3: 133:17479

REFERENCE 4: 130:52435

L23 ANSWER 123 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN **215238-12-3** REGISTRY

CN Benzamide, 4-[(1E)-3-[[2-[[2,4-dichloro-3-[[3-methyl-5-quinoxalinyloxy)methyl]phenyl)methylamino]-2-oxoethyl]amino]-3-oxo-1-propenyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C30 H27 Cl2 N5 O4 . Cl H

SR CA

LC STN Files: CA, CAPLUS, CASREACT

DT.CA Caplus document type: Journal

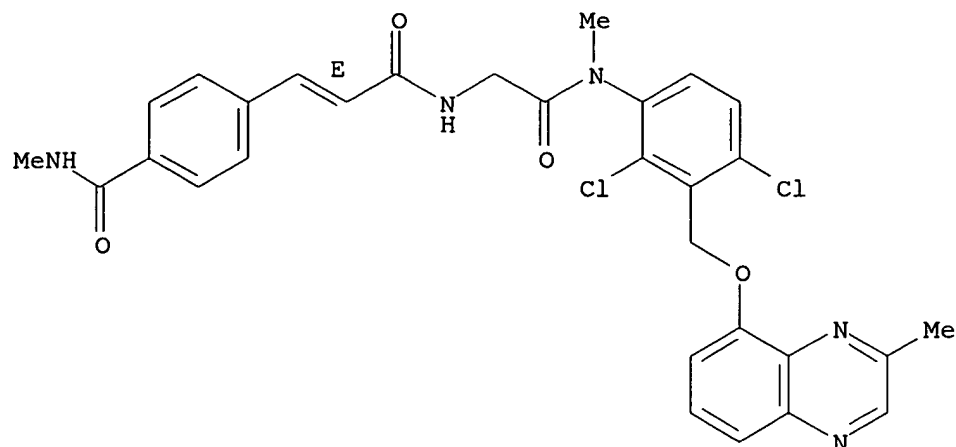
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

CRN (215238-10-1)

Double bond geometry as shown.

Searcher : Shears 571-272-2528

10/088814



● HCl

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:368093

REFERENCE 2: 129:325738

L23 ANSWER 124 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN **187479-26-1** REGISTRY

CN Phosphonic acid, [(1,2,3,4-tetrahydro-2,3-dioxo-5-quinoxaliny)methyl]-
(9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C9 H9 N2 O5 P

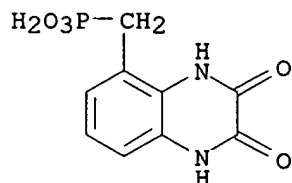
SR CA

LC STN Files: CA, CAPLUS, CASREACT

DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES
(Uses)

RL.NP Roles from non-patents: BIOL (Biological study); PRP (Properties); RACT
(Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Searcher : Shears 571-272-2528

10/088814

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:226178

REFERENCE 2: 126:186210

L23 ANSWER 126 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 168835-90-3 REGISTRY

CN 1,2-Benzenediol, 4-(6,7-dimethyl-2-quinoxaliny)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN AG 1433

CN SU 1433

FS 3D CONCORD

DR 197592-59-9

MF C16 H14 N2 O2

CI COM

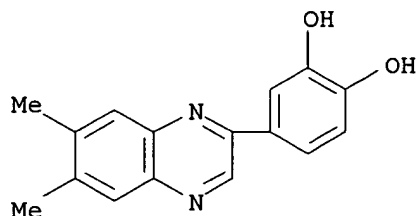
SR CA

LC STN Files: BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS, IMSDRUGNEWS,
IMSRESEARCH, TOXCENTER, USPATFULL

DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES
(Uses)

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation);
PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

14 REFERENCES IN FILE CA (1907 TO DATE)

14 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:270356

REFERENCE 2: 139:122710

REFERENCE 3: 139:106450

REFERENCE 4: 138:8422

REFERENCE 5: 136:53764

REFERENCE 6: 131:346563

Searcher : Shears 571-272-2528

10/088814

REFERENCE 7: 131:322425

REFERENCE 8: 129:175652

REFERENCE 9: 129:54393

REFERENCE 10: 128:154102

L23 ANSWER 127 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 91147-43-2 REGISTRY

CN 6-Quinoxalinamine, N-(4,5-dihydro-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN UK 41511

FS 3D CONCORD

MF C11 H11 N5

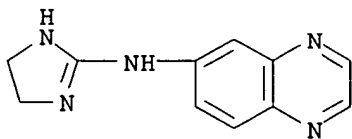
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); USES (Uses)

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

14 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

14 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:265771

REFERENCE 2: 138:226731

REFERENCE 3: 138:112477

REFERENCE 4: 137:358171

REFERENCE 5: 136:123675

REFERENCE 6: 136:6009

REFERENCE 7: 134:188222

REFERENCE 8: 133:89544

Searcher : Shears 571-272-2528

10/088814

REFERENCE 9: 123:329809

REFERENCE 10: 123:217719

L23 ANSWER 128 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 59803-98-4 REGISTRY

CN 6-Quinoxalinamine, 5-bromo-N-(4,5-dihydro-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 5-Bromo-6-(2-imidazolin-2-ylamino)quinoxaline

CN AGN 190342

CN Brimonidine

CN Bromoxidine

CN UK 14304

CN UK 14304-18

FS 3D CONCORD

DR 109826-55-3

MF C11 H10 Br N5

CI COM

LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CBNB, CHEMCATS, CIN, CSCHEM, DDFU, DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDB, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MEDLINE, MRCK*, PHAR, PROMT, PROUSDDR, PS, RTECS*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL, VETU

(*File contains numerically searchable property data)

Other Sources: WHO

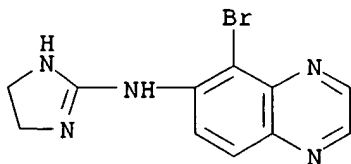
DT.CA Caplus document type: Conference; Journal; Patent

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)

RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PROC (Process); USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

RLD.NP Roles for non-specific derivatives from non-patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

719 REFERENCES IN FILE CA (1907 TO DATE)

8 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

721 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:86673

Searcher : Shears 571-272-2528

10/088814

REFERENCE 2: 142:69446
REFERENCE 3: 142:62657
REFERENCE 4: 142:49146
REFERENCE 5: 142:775
REFERENCE 6: 141:384335
REFERENCE 7: 141:361003
REFERENCE 8: 141:355430
REFERENCE 9: 141:355374
REFERENCE 10: 141:301455

L23 ANSWER 129 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 14121-55-2 REGISTRY

CN 6-Quinoxalinecarboxylic acid, 1,2,3,4-tetrahydro-2,3-dioxo- (7CI, 9CI)
(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 6-Quinoxalinecarboxylic acid, 2,3-dihydroxy- (8CI)

OTHER NAMES:

CN 2,3-Dihydroxy-6-quinoxalinecarboxylic acid

CN NSC 211121

FS 3D CONCORD

MF C9 H6 N2 O4

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST,
CSCHEM, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Other Sources: EINECS**

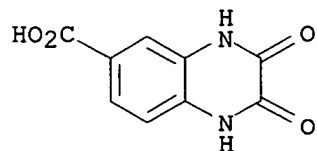
(**Enter CHEMLIST File for up-to-date regulatory information)

DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PROC
(Process); RACT (Reactant or reagent); USES (Uses); NORL (No role in
record)

RLD.P Roles for non-specific derivatives from patents: BIOL (Biological
study); USES (Uses)

RL.NP Roles from non-patents: BIOL (Biological study); CMBI (Combinatorial
study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

17 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

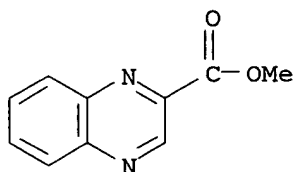
Searcher : Shears 571-272-2528

10/088814

17 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 139:240337
REFERENCE 2: 137:257239
REFERENCE 3: 136:210595
REFERENCE 4: 136:151182
REFERENCE 5: 133:4414
REFERENCE 6: 131:74941
REFERENCE 7: 122:108650
REFERENCE 8: 122:10070
REFERENCE 9: 118:182828
REFERENCE 10: 101:7194

L23 ANSWER 130 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN 1865-11-8 REGISTRY
CN 2-Quinoxalinecarboxylic acid, methyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H8 N2 O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, TOXCENTER
(*File contains numerically searchable property data)
DT.CA Caplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent); NORL (No role in record)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 142:93713
REFERENCE 2: 138:73233

Searcher : Shears 571-272-2528

REFERENCE 3: 136:274953

REFERENCE 4: 108:112059

REFERENCE 5: 94:208098

REFERENCE 6: 62:29499

REFERENCE 7: 54:133474

REFERENCE 8: 54:133473

REFERENCE 9: 54:133472

L23 ANSWER 131 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN

RN 91-19-0 REGISTRY

CN Quinoxaline (8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1,4-Benzodiazine

CN 1,4-Diazanaphthalene

CN 1,4-Naphthyridine

CN Benzoparadiazine

CN Benzopyrazine

CN Benzo[a]pyrazine

CN Phenopiazine

CN Phenpiazine

CN Quinazine

FS 3D CONCORD

MF C8 H6 N2

CI COM, RPS

LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DETHERM*, EMBASE, GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, TULSA, USPAT2, USPATFULL

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

DT.CA Caplus document type: Book; Conference; Dissertation; Journal; Patent; Preprint; Report

RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

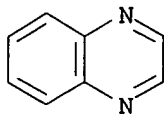
RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)

RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process);

10/088814

PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1875 REFERENCES IN FILE CA (1907 TO DATE)
579 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1878 REFERENCES IN FILE CAPLUS (1907 TO DATE)
22 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 142:120589
REFERENCE 2: 142:114039
REFERENCE 3: 142:113926
REFERENCE 4: 142:102844
REFERENCE 5: 142:93707
REFERENCE 6: 141:418065
REFERENCE 7: 141:416008
REFERENCE 8: 141:403674
REFERENCE 9: 141:366582
REFERENCE 10: 141:366136

FILE 'CAOLD' ENTERED AT 09:59:39 ON 07 FEB 2005
L24 26 S L23

L24 ANSWER 1 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA65:20778a CAOLD
TI microbiocidal compns. derived from quinoxaline
AU Hattori, Junnosuke; Koike, S.; Ozaki, T.; Yoshioka, H.; Sugiyama, H.
DT Patent
TI quinoxaline, microbiocidal compns. derived from
PA Sumitomo Chemical Co., Ltd.
DT Patent

	PATENT NO.	KIND	DATE
PI	GB 1043042		
IT	91-19-0	2075-99-2	2347-47-9 13313-95-6

L24 ANSWER 2 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA65:16097f CAOLD
TI thin-layer chromatography of azines and of aromatic N heterocycles on

Searcher : Shears 571-272-2528

Al203

AU Klemm, LeRoy H.; Klopfenstein, C. E.; Kelly, H. P.
 IT 85-02-9 91-19-0 91-62-3 91-63-4 92-82-0
 103-30-0 119-65-3 119-91-5 207-11-4 215-64-5 217-68-5
 225-02-5 225-06-9 225-51-4 229-87-8 230-17-1 230-27-3
 230-46-6 238-06-2 244-99-5 253-52-1 253-66-7 254-79-5
 260-94-6 272-67-3 366-18-7 484-11-7 491-35-0 538-49-8
 588-68-1 602-56-2 611-32-5 612-60-2 613-15-0 729-43-1
 826-77-7 877-43-0 939-23-1 1008-89-5 1125-80-0 1135-32-6
 1198-37-4 1437-15-6 1463-17-8 1630-53-1 1684-14-6 1721-93-3
 1759-29-1 1759-30-4 2071-44-5 2144-00-5 2379-55-7 2633-06-9
 3002-81-1 3248-05-3 4559-60-8 4594-84-7 5097-91-6 5097-93-8
 6957-19-3 6957-22-8 6957-24-0 7153-23-3 13341-40-7 13362-54-4
 13362-55-5 13362-56-6 13362-58-8 13362-59-9 13362-63-5 13362-71-5
 13362-75-9 13362-77-1 13362-78-2 13362-80-6 13362-81-7 13362-83-9
 14722-38-4 89939-13-9 92552-20-0

L24 ANSWER 3 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
 AN CA65:13186h CAOLD
 TI transition-metal quinoxaline complexes - (III) Cu(II) derivs. with
 substituted quinoxalines
 AU Billing, D. E.; Underhill, A. E.; Adams, D. M.; Morris, D. M.
 IT 91-19-0 1684-14-6 2379-55-7 7251-61-8 14284-58-3
 14376-51-3 26316-88-1 26316-89-2 36005-76-2 94006-95-8 94502-35-9
 101546-44-5 101546-46-7

L24 ANSWER 4 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
 AN CA65:7307a CAOLD
 TI polymerization of acetylenic hydrocarbons
 AU Dubeck, Michael; Filbey, A. H.
 PA Ethyl Corp.
 DT Patent
 PATENT NO. KIND DATE

 PI US 3256260 1966
 IT 91-19-0 92-82-0 107-19-7 229-87-8 230-07-9
 253-52-1 253-66-7 253-82-7 288-13-1 288-32-4 288-36-8
 289-80-5 289-96-3 290-37-9 290-38-0 471-25-0 557-12-0
 557-19-7 627-19-0 1271-28-9 1293-95-4 1932-93-0 12071-73-7
 12087-67-1 14220-17-8 14653-44-2 14917-13-6 14917-14-7 14917-15-8
 15625-54-4 15793-12-1 31811-17-3 52445-55-3

L24 ANSWER 5 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
 AN CA65:7004b CAOLD
 TI radical phenylation of bicyclic heterocyclic compds.
 AU Dou, Henri J. M.; Lynch, B. M.
 IT 91-19-0 95-16-9 1632-83-3

L24 ANSWER 6 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
 AN CA65:2646a CAOLD
 TI nitrogenous heterocycles in cigaret smoke condensate
 AU Testa, Albert; Testa, P.
 IT 91-19-0 290-37-9

L24 ANSWER 7 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
 AN CA64:18711c CAOLD

10/088814

TI far-ultraviolet spectra of azines in solution
AU Favini, Giorgio; Bellobono, I. R.
IT 91-19-0 253-52-1 253-66-7 253-82-7 289-80-5
290-37-9 290-87-9

L24 ANSWER 8 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:10625e CAOLD
TI 14N hyperfine structure in electron spin resonance spectra of heterocyclic
anions
AU Henning, J. C. M.
IT 91-19-0 92-82-0 254-79-5 289-80-5 290-37-9
6918-15-6 89939-13-9

L24 ANSWER 9 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:10608e CAOLD
TI measurement of the polarization of the phosphorescence of certain diazines
in vitreous solution at 77°K. and interpretation of the results by
spin-orbit interaction
AU Loustauneau, Pierre
IT 91-19-0 290-37-9

L24 ANSWER 10 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:10600g CAOLD
TI singlet-singlet and triplet-triplet absorption spectra of certain diazines
in crystallized solns.
AU Loustauneau, Pierre; Nouchi, G.
IT 91-19-0 92-82-0

L24 ANSWER 11 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:10547b CAOLD
TI magnetophotoselection of the lowest excited triplet state of aromatic
mols.
AU El-Sayed, Mostafa A.; Siegel, S.
IT 91-19-0 538-04-5 1146-65-2 1517-22-2

L24 ANSWER 12 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:9574d CAOLD
TI inductive and mesomeric effects in substituted organic mols. - (XX) pyrazine
derivs.
AU Lumbroso, Henri; Palamidessi, G.
IT 91-19-0 1628-89-3

L24 ANSWER 13 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:9117c CAOLD
TI heterogeneous catalysis by organic conjugated polymers-electron spin
resonance and structural factors
AU Gallard-Nechtschein, Jacqueline; Laederich, T.; Nechtschein, M.; Pecher,
A.; Salle, R.; Traynard, P.
IT 51-17-2 91-19-0 32518-77-7

L24 ANSWER 14 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:9073c CAOLD
TI azanaphthalenes - (I) Hueckel orbital calcns.
AU Wait, Samuel C., Jr.; Wesley, J. W.
IT 91-18-9 91-19-0 253-45-2 253-50-9 253-52-1
253-61-2 253-66-7 253-69-0 253-72-5 253-74-7 253-82-7

Searcher : Shears 571-272-2528

10/088814

253-83-8	253-86-1	253-87-2	253-88-3	254-60-4	254-61-5
254-62-6	254-79-5	254-80-8	254-81-9	254-82-0	254-83-1
254-86-4	254-87-5	254-91-1	254-95-5	254-96-6	254-97-7
254-99-9	255-00-5	255-01-6	255-53-8	322-46-3	767-95-3
6133-37-5	6133-39-7	6133-40-0	6133-43-3	6133-44-4	6133-45-5
6133-46-6	6133-50-2	6133-56-8	6133-57-9	6133-58-0	6133-59-1
6133-60-4	6133-64-8	6133-65-9	6133-66-0	6133-67-1	6133-68-2
6133-69-3	6133-70-6	6133-71-7	6133-72-8	6133-73-9	6133-75-1
6133-76-2	6133-77-3	6133-78-4	6133-79-5	6133-80-8	6133-96-6
6133-97-7	6133-98-8	6133-99-9	6380-84-3	7666-88-8	89939-13-9

L24 ANSWER 15 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:7535h CAOLD
TI infrared spectra of some diaza- and triazanaphthalenes and of
1,4,5,8-tetraazanaphthalene
AU Armarego, W. L. F.; Barlin, G. B.; Spinner, E.
DT Patent
IT 91-19-0 253-82-7 254-79-5 255-53-8 14336-94-8
14380-59-7

L24 ANSWER 16 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA63:17326g CAOLD
TI calcn. of electronic spectra of azabenzenes and azanaphthalenes by the
Pariser-Parr-Pople method
AU Favini, Giorgio; Vandoni, I.; Simonetta, M.
IT 91-18-9 91-19-0 253-45-2 253-52-1 253-66-7
253-69-0 253-72-5 253-82-7 253-86-1 253-87-2 254-60-4
254-61-5 254-79-5 254-80-8 254-86-4 254-87-5 255-53-8
289-96-3 290-37-9 290-38-0 290-42-6 290-87-9 290-96-0
322-46-3 592-59-6 89939-13-9

L24 ANSWER 17 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA63:10883b CAOLD
TI analysis of the proton nuclear magnetic resonance spectra of
heteroaromatic systems - (V) diazanaphthalenes
AU Black, Peter J.; Heffernan, M. L.
IT 91-19-0 253-52-1 253-66-7 253-82-7

L24 ANSWER 18 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA63:1353d CAOLD
TI spectroscopy and photosensitization of various photochromic spiropyrans
AU Becker, Ralph S.; Roy, J. K.
IT 91-19-0 1485-92-3 1498-88-0 1498-89-1 1592-43-4

L24 ANSWER 19 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA63:168c CAOLD
TI shifts and electron ds. in N heterocyclic mols.
AU Gawer, Albert; Dailey, B. P.
IT 91-19-0 253-52-1 253-66-7 253-82-7 254-79-5
289-80-5 290-37-9 12015-14-4 89939-13-9

L24 ANSWER 20 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA63:36b CAOLD
TI zero-field splittings - (V) aromatic N heterocycles
AU Boorstein, Seth A.; Gouterman, M.
IT 91-19-0 290-37-9

Searcher : Shears 571-272-2528

L24 ANSWER 21 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
 AN CA62:14062c CAOLD
 TI luminescence and the triplet state
 AU Rousset, Auguste
 IT 91-19-0 92-82-0 290-37-9

L24 ANSWER 22 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
 AN CA62:11833f CAOLD
 TI nitrofuran derivs. having a triazine ring
 AU Kodama, Yutaka; Takai, A.; Saikawa, I.; Haseda, M.
 PA Toyama Chemical Industry Co., Ltd.
 DT Patent

	PATENT NO.	KIND	DATE			
PI	JP 64028256		1964			
IT	842-81-9	893-25-4	893-26-5	895-65-8	900-70-9	952-11-4
	14121-55-2					

L24 ANSWER 23 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
 AN CA62:8525f CAOLD
 TI calcn. of electronic spectra of azabenzenes and azanaphthalenes by the Pariser-Parr-Pople method

AU Favini, Giorgio; Vandoni, I.; Simonetta, M.
 IT 91-18-9 91-19-0 253-45-2 253-50-9 253-52-1
 253-66-7 253-69-0 253-72-5 253-82-7 253-86-1 253-87-2
 254-60-4 254-61-5 254-79-5 254-80-8 254-86-4 254-87-5
 255-53-8 289-80-5 289-96-3 290-37-9 290-38-0 290-42-6
 290-87-9 290-96-0 322-46-3 592-59-6 89939-13-9

L24 ANSWER 24 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
 AN CA62:5215c CAOLD

TI basic cleavages of arylsulfonamides
 AU Negishi, Eiichi; Day, A. R.
 IT 1096-43-1 1865-09-4 1865-10-7 1865-11-8 1865-12-9
 1865-13-0 1865-14-1 1865-15-2 1865-16-3 1865-18-5 1865-19-6
 2101-20-4 2101-21-5 2680-41-3 2762-31-4 3442-30-6 3442-50-0
 3753-91-1 4092-09-5 4099-43-8 63068-63-3 105042-90-8

L24 ANSWER 25 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
 AN CA54:25560a CAOLD

TI antibiotics from Streptomyces
 AU Prelog, Vladimir; Gaeumann, E.; Wettstein, A.
 DT Patent
 TI proteolytic enzyme
 PA American Cyanamid Co.
 DT Patent

	PATENT NO.	KIND	DATE
PI	DE 1025572		
IT	879-65-2	1865-11-8	

L24 ANSWER 26 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
 AN CA52:6361h CAOLD
 TI phenazines - (XV) ring cleavage of phenazine(1) 2,3-quinoxalinediacarboxylic acid

10/088814

AU Yoshioka, Ichiro; Otomasu, H.
IT 1865-11-8 2876-17-7 2876-18-8 5182-90-1 5660-34-4
6924-99-8 54571-06-1 110490-03-4

FILE 'USPATFULL' ENTERED AT 10:00:01 ON 07 FEB 2005

L25 270 SEA ABB=ON PLU=ON L23
L26 0 SEA ABB=ON PLU=ON L23(L) (PHARM? OR DRUG OR PRODRUG OR
MEDICIN## OR MEDICAT?)

L29 0 SEA ABB=ON PLU=ON L23(L) (PREP? OR PRODUCING OR PRODUCE# OR
PRODUCTION OR MANUF?)

L30 0 SEA ABB=ON PLU=ON L23(L) (METHOD OR TECHNIQUE)

(FILE 'MEDLINE, BIOSIS, EMBASE' ENTERED AT 10:03:05 ON 07 FEB 2005)

L32 4089 SEA ABB=ON PLU=ON L23
L33 0 SEA ABB=ON PLU=ON L32(L) (PHARM? OR DRUG OR PRODRUG OR
MEDICIN## OR MEDICAT?)

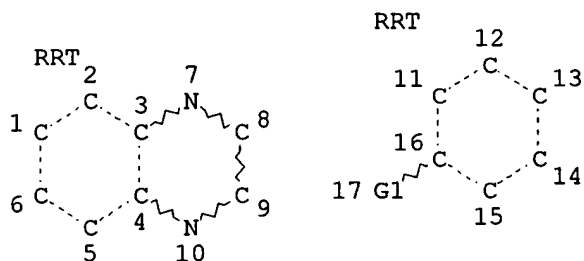
L40 0 S L32(L) (METHOD OR TECHNIQUE)

L41 0 S L32(L) (TREAT? OR THERAP?)

L42 0 SEA ABB=ON PLU=ON L32(L) (PREP? OR PRODUCING OR PRODUCE# OR
PRODUCTION OR PROD## OR MANUF?)

(FILE 'CASREACT' ENTERED AT 10:30:38 ON 07 FEB 2005)

L46 STR



VAR G1=SH/NH/OH

NODE ATTRIBUTES:

CONNECT IS X2 RC AT 7

CONNECT IS X2 RC AT 10

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

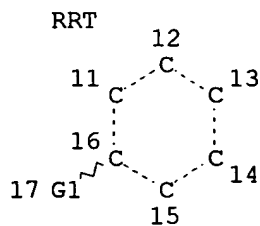
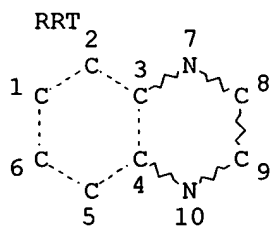
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

L48 276 SEA FILE=CASREACT SSS FUL L46 (2173 REACTIONS)

L53 STR

10/088814



PRO

Hy~G2~Cb~NH~G3
18 19 20 21 22

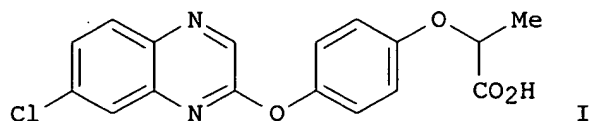
VAR G1=SH/NH/OH
VAR G2=O/S/N
VAR G3=C/S
NODE ATTRIBUTES:
CONNECT IS X2 RC AT 7
CONNECT IS X2 RC AT 10
DEFAULT MLEVEL IS ATOM
GGCAT IS PCY UNS AT 18
GGCAT IS UNS AT 20
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E2 N AT 18

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE
L54 1 SEA FILE=CASREACT SUB=L48 SSS FUL L53 (5 REACTIONS)
100.0% DONE 2169 VERIFIED 5 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

L54 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 135:76849 CASREACT
TITLE: Design, Synthesis, and Biological Evaluation of Analogues of the Antitumor Agent, 2-(4-[(7-Chloro-2-quinoxalinyloxy)phenoxy]propionic Acid (XK469)
AUTHOR(S): Hazeldine, Stuart T.; Polin, Lisa; Kushner, Juiwanna; Paluch, Jennifer; White, Kathryn; Edelstein, Matthew; Palomino, Eduardo; Corbett, Thomas H.; Horwitz, Jerome P.
CORPORATE SOURCE: Department of Internal Medicine Division of Hematology and Oncology, Wayne State University School of Medicine, Detroit, MI, 48201, USA
SOURCE: Journal of Medicinal Chemistry (2001), 44(11), 1758-1776
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

Searcher : Shears 571-272-2528



AB 2-(4-[(7-Chloro-2-quinoxalinyloxy]phenoxy)propionic acid (XK469) I is among the most highly and broadly active antitumor agents to have been evaluated and scheduled to enter clin. trials in 2001. The mechanism or mechanisms of action of I remain to be elaborated. Accordingly, an effort was initiated to establish a pharmacophore hypothesis to delineate the requirements of the active site, via a comprehensive program of synthesis of analogs of I and evaluation of the effects of structural modification(s) on solid tumor activity. The strategy formulated chose to dissect the two-dimensional parent structure into three regions: I, ring A of quinoxaline; II, the hydroquinone connector linkage; and III, the lactic acid moiety-to determine the resultant in vitro and in vivo effects

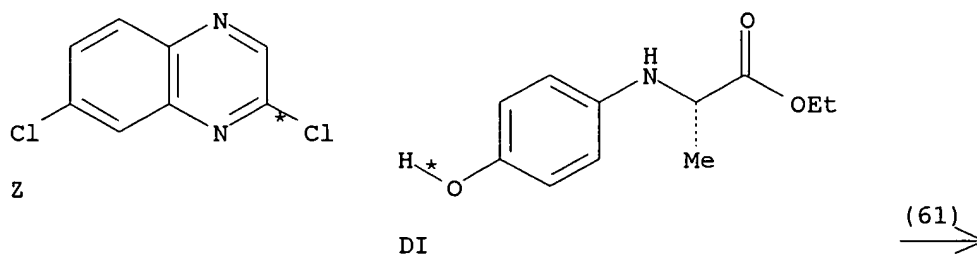
of

chemical alterations in each region. Neither the A-ring unsubstituted nor the B-ring 3-chloro-regioisomer of I showed antitumor activity. The modulating antitumor effect(s) of substituents of differing electronegativities, located at the several sites comprising the A-ring of region I, were next ascertained. Thus, a halogen substituent, located at the 7-position of a 2-(4-[(2-quinoxalinyloxy]phenoxy)propionic acid, generated the most highly and broadly active antitumor agents. A Me, methoxy, or an azido substituent at this site generated a much less active structure, whereas 5-, 6-, 8-chloro-, 6-, 7-nitro, and 7-amino derivs. all proved to be essentially inactive. When the connector linkage (region II) of I was changed from that of a hydroquinone to either a resorcinol or a catechol derivative, all antitumor activity was lost. Of the carboxylic

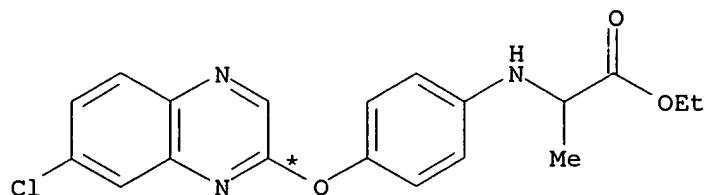
acid

derivs. of I (region III), i.e., CONH₂, CONHMe, CONMe₂, CONHOH, CONHNH₂, CN, or CN₄H (tetrazole), only the monomethyl- and N,N-dimethylamides proved to be active.

RX(61) OF 233 ...Z + DI ==> DO...



10/088814



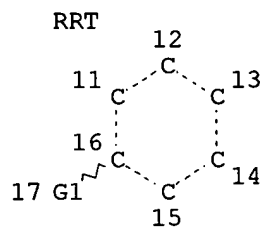
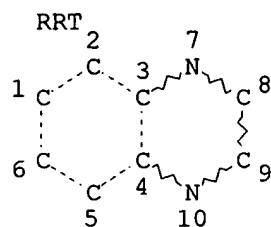
DO
YIELD 84%

RX(61) RCT Z 59489-31-5, DI 35897-44-0
RGT BL 584-08-7 K2CO3
PRO DO 347162-61-2
SOL 75-05-8 MeCN

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

(FILE 'DJSMDs, CHEMINFORMRX' ENTERED AT 10:38:02 ON 07 FEB 2005)

L51 STR



Hy G2 Cb
18 19 20

VAR G1=SH/NH/OH
VAR G2=O/S/N
NODE ATTRIBUTES:
CONNECT IS X2 RC AT 7
CONNECT IS X2 RC AT 10
DEFAULT MLEVEL IS ATOM
GGCAT IS PCY UNS AT 18
GGCAT IS UNS AT 20
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E2 N AT 18

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 20

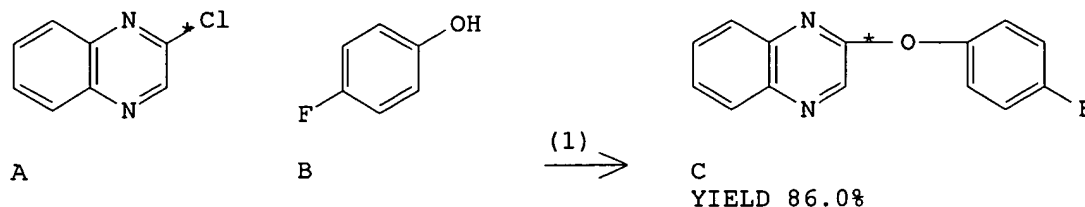
STEREO ATTRIBUTES: NONE
L55 14 SEA L51

L55 ANSWER 1 OF 14 DJSMDs COPYRIGHT 2005 THE THOMSON CORP on STN
AN 1999:1059 DJSMDs
TI 2-ARYLOXY- FROM 2-CHLORO-QUINOXALINES AND PHENOLS
AU Cuenca, A.
SO Synth Commun, 29(8), p.1393-9 (1999)

Searcher : Shears 571-272-2528

CODEN: SYNCAV ISSN: 0039-7911
 DT Journal
 VI 25-5
 AB Cf. 1987:76525C. The method is simple, mild and starting materials are accessible. Higher temperatures and longer reaction times are required for the reaction to proceed in the absence of silver nitrate. Cf. 1998:1052. For further examples, (74-83%), see citation 1.

RX(1) OF 1 A + B ==> C

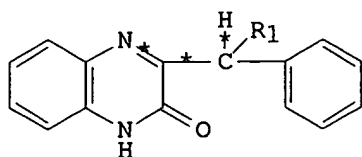


RX(1) RCT A, 13976
 B, 5784; 1 Eq.
 SOL 23, DMF
 CAT 879, AgNO₃; 10 mol. %
 135, KOH; 1 Eq.
 PRO C, 103447
 T 68.0 Cel
 TIM 1.0 hr
 CMT Path A

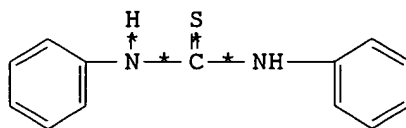
L55 ANSWER 2 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
 AN 200446155 CHEMINFORMRX
 TI Fused Polycyclic Nitrogen-Containing Heterocycles. Part 7. Reaction Products of 3-(α -Chlorobenzyl)-1,2-dihydroquinoxalin-2-one and Thioureas as Key Intermediate Compounds in the Synthesis of Thiazolo[3,4-a]quinoxalines.
 AU KALININ, A. A.; MAMEDOV, V. A.; RIZVANOV, I. K.; LEVIN, Y. A.
 CS Arbuzov Inst. Org. Phys. Chem., Kazan Res. Cent., Russ. Acad. Sci., Kazan' 420088, Russia
 SO Russ. J. Org. Chem., 40(4), 527-533 (2004)
 CODEN: RJOCEQ ISSN: 1070-4280
 LA English
 AB Quinoxalinone derivative (I) is subjected to reactions with reagents which are equivalents of the NCS species, in particular with (II), (V), 2-sulfanylbenzimidazole, and 2-sulfanylbenzothiazole. Attempted intramolecular cyclization reactions of the latter compounds fail. Heating thiourea (II) or N,N'-diphenylthiourea (VI) with quinoxalinone (I) in dioxane with subsequent addition of acetic anhydride affords the thiazoloquinoxalines (IV) and (VII). Unfortunately, the yield of (IV) for this one-pot procedure is considerably lower than in the two-step synthesis via isothioureide (V). Also, structures containing no heterocyclic system can be regarded as precursors of the title compounds. For example, synthetic equivalents for the required synthons are chloropyruvate (VIII), potassium thiocyanate (IX), and o-phenylenediamine (X).

RX(4) OF 6 A + I ==> J

10/088814

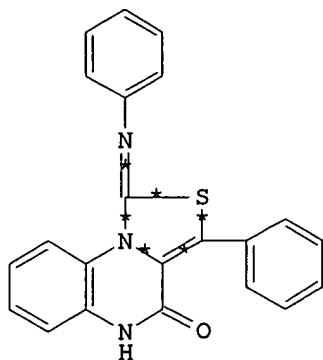


I



VI

(4) →



VII

YIELD 10.0%

RX(4) RCT I, **764252**
 VI, **34607** (102-08-9)
 STAGE(1)
 SOL 80 (123-91-1), dioxane
 T.KW REFLUX
 STAGE(2)
 RGT 4 (108-24-7), Ac2O
 3 (64-19-7), AcOH
 T.KW REFLUX
 PRO VII, **507274**
 YDS 10.0 %
 KW addition; alkylation; N-alkylation; S-alkylation
 NTE reaction:I 1.(VI) -> VII

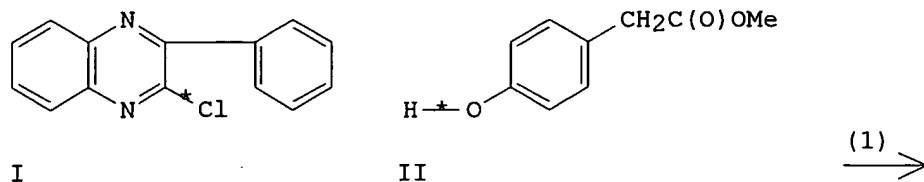
L55 ANSWER 3 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
 AN 200427140 CHEMINFORMRX
 TI Quinoxaline Chemistry. Part 17. Methyl [4-(Substituted-2-
 quinoxalinyloxy)phenyl]acetates and Ethyl N-([4-(Substituted-2-
 quinoxalinyloxy)phenyl]acetyl)glutamates Analogues of Methotrexate:

Searcher : Shears 571-272-2528

10/088814

Synthesis and Evaluation of in vitro Anticancer Activity.
AU PIRAS, S.; LORIGA, M.; PAGLIETTI, G.
CS Dip. Farm. Chim. Tossicol., Univ. Sassari, I-07100 Sassari, Italy
SO Farmaco, 59(3), 185-194 (2004)
CODEN: FRMCE8 ISSN: 0014-827X
LA English
AB Compounds (VII) and (VIb) show the strongest anticancer activity of all tested compounds.

RX(1) OF 18 A + B ==> C...



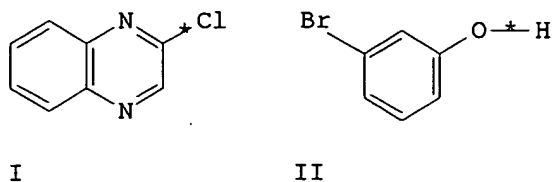
III
YIELD 90.0%

RX(1) RCT I, **391494**
II, **468959** (14199-15-6)
RGT 1042 (534-17-8), Cs2CO3
SOL 76 (68-12-2), DMF
PRO III, **1021305**
YDS 90.0 %
T 70.0 Cel
KW arylation; O-arylation; etherification
NTE reaction:I (II) -> III, example: 1

L55 ANSWER 4 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 200231171 CHEMINFORMRX
TI Silver(I)-Catalyzed Synthesis of Novel Quinoxaline Derivatives.
AU RIZZO, A.; CAMPOS, G.; ALVAREZ, A.; CUENCA, A.
CS Dep. Quim., Univ. Simon Bolivar, Caracas 1080-A, Venez.
SO Synth. Commun., 32(5), 813-817 (2002)
CODEN: SYNCAV ISSN: 0039-7911
LA English
AB The reaction of chloroquinoxaline (I) with phenoxide ion derivatives (II) utilizing Ag+ as catalyst provides an excellent method for the preparation of the title compounds (III).

RX(1) OF 4 A + B ==> C

10/088814

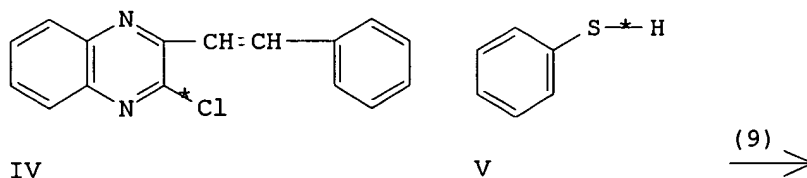


III
YIELD 68.0%

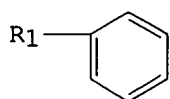
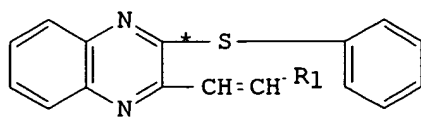
RX(1) RCT I, **157891** (1448-87-9)
II, **22002** (591-20-8)
RGT 1160 (1310-58-3), KOH
SOL 76 (68-12-2), DMF
CAT 1177 (7761-88-8), AgNO₃
PRO III, **890723**
YDS 68.0 %
T 70.0 - 81.0 Cel
KW arylation; O-arylation; etherification
NTE reaction:I (II) -> III, example: 1

L55 ANSWER 5 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 200140147 CHEMINFORMRX
TI Studies on the Synthesis of 2-Phenylsulfonyl-3-styrylquinoxalines.
AU KRISHNAN, V. S. H.; CHOWDARY, K. S.; DUBEY, P. K.; VIJAYA, S.
CS Dep. Chem., Coll. Eng., JNT Univ., Kukatpally 500 072, India
SO Indian J. Chem., Sect. B: Org. Chem. Incl. Med. Chem., 40(7), 565-573 (2001)
CODEN: IJSBDB ISSN: 0376-4699
LA English
AB Several variations of a synthetic pathway to the title compounds (VII) starting from 3-methylbenzo-1H-dihydropyrazine-2-one (I) are described.

RX(9) OF 52 ...K + Q ==> R...



10/088814

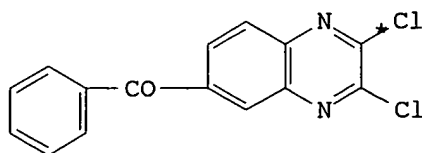


VI
YIELD 95.0%

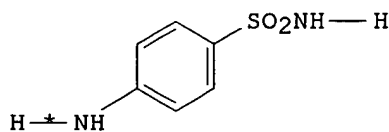
RX(9) RCT IV, **834480**
V, **211** (108-98-5)
RGT 216 (121-44-8), Et3N
SOL 123 (67-56-1), MeOH
PRO VI, **834484**
YDS 95.0 %
T.KW REFLUX
KW arylation
NTE reaction:IV (V) -> VI, example: 1

L55 ANSWER 6 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 200126156 CHEMINFORMRX
TI Some Nucleophilic Reactions with 6-Benzoyl-2,3-dichloroquinoxaline:
Synthesis of Tetrazolo[1,5-a]quinoxaline, 2-Methylidene-1,3-dithiolo[4,5-b]quinoxalines, Quinoxalino[2,3-b]quinoxalines and
Pyrazolo[1',5':1,2]imidazolo[4,5-b]quinoxalines.
AU EL-GABY, M. S. A.; EL-SHARIEF, A. M. S.; AMMAR, Y. A.; MOHAMED, Y. A.;
EL-SALAM, A. A. A.
CS Dep. Chem., Fac. Sci., Al-Azhar Univ., Assuit 71524, Egypt
SO Indian J. Chem., Sect. B: Org. Chem. Incl. Med. Chem., 40(3), 195-200
(2001)
CODEN: IJSBDB ISSN: 0376-4699
LA English
AB The starting compound (I) is subjected to some nucleophilic reagents to
study the effect of the benzoyl group on the reactivity of the two
chlorine atoms.

RX(2) OF 11 A + E ==> F



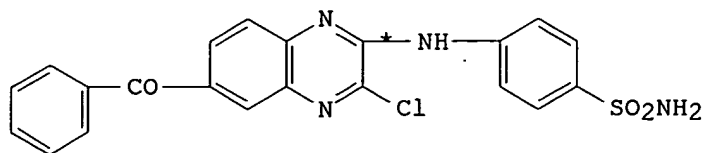
I



II

(2) →

10/088814

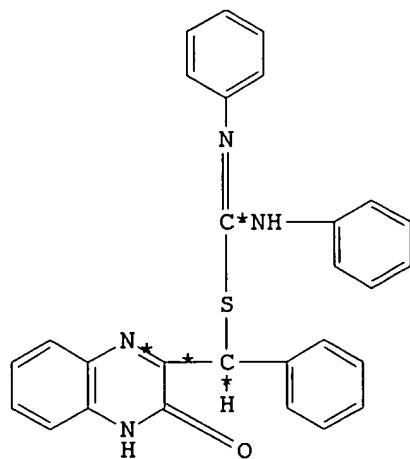


III
YIELD 60.0%

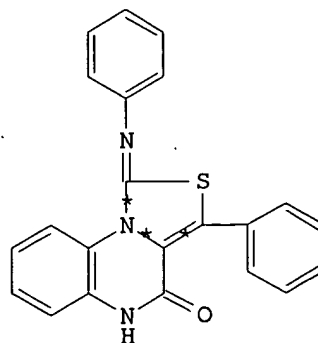
RX(2) RCT I, 85308 (143702-67-4)
II, 19559 (63-74-1)
SOL 76 (68-12-2), DMF
PRO III, 814530
YDS 60.0 %
T.KW REFLUX
KW arylation
NTE reaction:I (II) -> III, example: 2

L55 ANSWER 7 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 200037168 CHEMINFORMRX
TI 3-Aryl-1-imino-4-oxo-4,5-dihydrothiazolo[3,4-a]quinoxalines.
Retrosynthetic Approach.
AU MAMEDOV, V. A.; KALININ, A. A.; GUBAIDULLIN, A. T.; NURKHAMETOVA, I. Z.;
LITVINOV, I. A.; LEVIN, Y. A.
CS Arbuzov Inst. Org. Phys. Chem., Kazan Sci. Cent., Russ. Acad. Sci., Kazan
420088, Russia
SO Chem. Heterocycl. Compd. (N. Y.), 35(12), 1459-1473 (1999)
CODEN: CHCCAL ISSN: 0009-3122
LA English
AB Methods for constructing fused thiazoloquinoxaline systems such as (IV)
and (VII) from 3-(α -chlorobenzyl)quinoxalinones (I) via the
intermediacy of corresponding 3-(α -thiocyanatobenzyl)- and
3-(α -isothioureidobenzyl) derivatives are developed.

RX(6) OF 9 ...K ==> L



VI



VII
YIELD 33.0%

Searcher : Shears 571-272-2528

10/088814

RX(6) RCT VI, **764257**
SOL 3 (64-19-7), AcOH
PRO VII, **507274**
YDS 33.0 %
T.KW REFLUX
KW alkylation; N-alkylation
NTE reaction:VI -> VII

L55 ANSWER 8 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN

AN 199922160 CHEMINFORMRX

TI Quinoxaline Chemistry. Part 12. 3-Carboxy-2[phenoxy]-6(7) Substituted Quinoxalines and N-[4-(6(7) Substituted-3-carboxyquinoxalin-2-yl)hydroxy] Benzoylglutamates. Synthesis and Evaluation of in vitro Anticancer Activity.

AU VITALE, G.; CORONA, P.; LORIGA, M.; PAGLIETTI, G.

CS Ist. Chim. Farm. Tossicol., Univ. Sassari, I-07100 Sassari, Italy

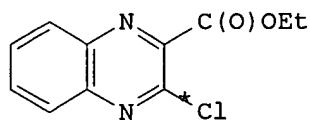
SO Farmaco, 53(8), 594-601 (1998)

CODEN: FRMCE8 ISSN: 0014-827X

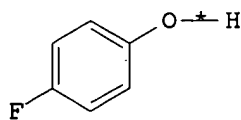
LA English

AB Thirty quinoxalines, bearing a substituted phenoxy or hydroxybenzoylglutamate group in position 2, are prepared in order to evaluate the in vitro anticancer activity. Screening reveals that only few derivatives, e.g. (IIIc) and (IIId), exhibit moderate growth inhibition activity on various tumor panel cell lines.

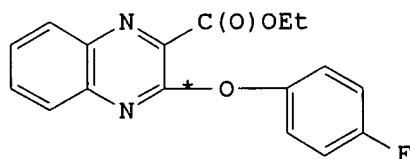
RX(1) OF 9 A + B ==> C



I



II



III

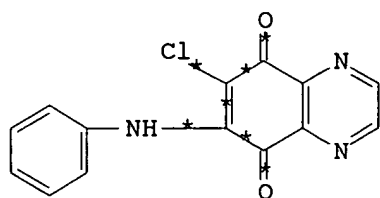
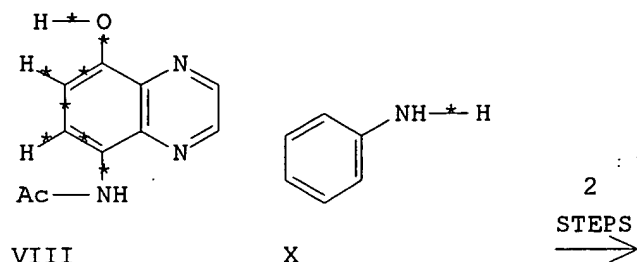
YIELD 67.0%

RX(1) RCT I, **200473** (49679-45-0)
II, **12611** (371-41-5)
RGT 1042 (534-17-8), Cs2CO3
SOL 76 (68-12-2), DMF
PRO III, **673122**
YDS 67.0 %
T 70.0 Cel
KW arylation; O-arylation; etherification
NTE reaction:I (II) -> III, example: 1

Searcher : Shears 571-272-2528

L55 ANSWER 9 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
 AN 199712148 CHEMINFORMRX
 TI A New Synthetic Route to 6,7-Dichloro-5,8-quinoxalinedione and Synthesis of Its Derivatives.
 AU HAN, G.; SHIN, K. J.; KIM, D. C.; YOO, K. H.; KIM, D. J.; PARK, S. W.
 CS Div. Appl. Sci., Korea Inst. Sci. Technol., Seoul 131-650, S. Korea
 SO Heterocycles, 43(11), 2495-2502 (1996)
 CODEN: HTCYAM ISSN: 0385-5414
 LA English
 AB The title compound (IX) is prepared from 4-aminophenol (I) in 8 steps. Key step of the sequence is the chloroxidation of the intermediate sulfate obtained from (VIII). The reaction of (IX) with a variety of nitrogen nucleophiles is investigated.

RX(15) OF 42 COMPOSED OF RX(6), RX(7)
 RX(15) M + V ==> W



YIELD 81.0%

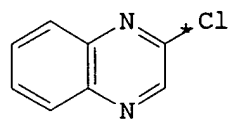
RX(6) RCT VIII, 520407
 STAGE(1)
 RGT 198 (7664-93-9), H2SO4
 STAGE(2)
 RGT 1338 (7775-09-9), NaClO3
 103 (7647-01-0), HCl
 T 0.0 Cel
 PRO IX, 520408
 YDS 63.0 %
 KW dearomatisation; halogenation; C-halogenation; chlorination;
 alkylation
 NTE reaction:VIII -> IX
 RX(7) RCT IX, 520408
 X, 13 (62-53-3)

10/088814

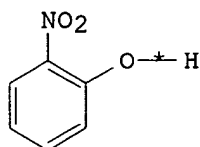
RGT 318 (7790-86-5), CeCl₃
SOL 6 (75-05-8), MeCN
PRO XI, **520409**
YDS 81.0 %
T 25.0 Cel
KW alkylation; N-alkylation
NTE reaction:IX (X) -> XI

L55 ANSWER 10 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 199652180 CHEMINFORMRX
TI Synthesis of 2-(2-Nitrophenoxy)quinoxaline and Its Basic Hydrolysis in Aqueous Solutions of Non-Reactive Counter-Ion Surfactants with Bulky Head Groups.
AU CUENCA, A.; STRUBINGER, A.
CS Dep. Quim., Univ. Simon Bolivar, Caracas 1080-A, Venez.
SO Tetrahedron, 52(36), 11665-11672 (1996)
CODEN: TETRAB ISSN: 0040-4020
LA English
AB Micellar effects upon the reaction of hydroxide ions with the title compound (III) are analyzed and the effect of the micellar head group size upon the reaction is investigated. As surfactants cetyltrialkylammonium salts are used. The kinetic data reveal that the basic hydrolysis of (III) to the quinoxalone (IV) can be explained by assuming independent equilibrium distribution for ions in solution between aqueous and micellar pseudophases.

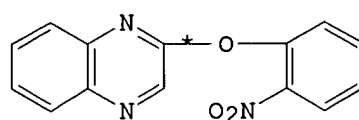
RX(1) OF 1 A + B ==> C



I



II



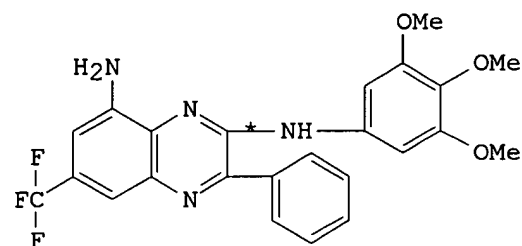
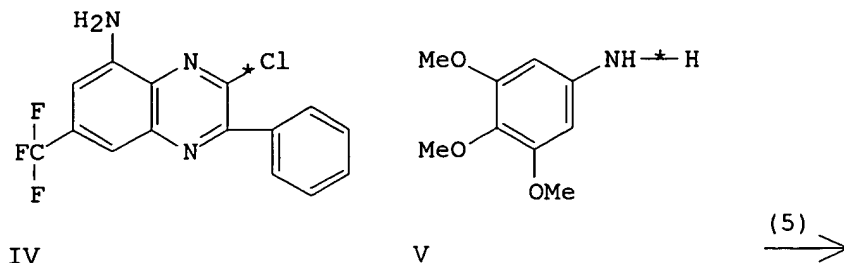
III
YIELD 77.0%

RX(1) RCT I, **157891** (1448-87-9)
II, **16226** (88-75-5)
RGT 1160 (1310-58-3), KOH
SOL 76 (68-12-2), DMF
PRO III, **505676**
YDS 77.0 %
T.KW REFLUX
KW arylation; O-arylation; etherification
NTE reaction:I (II) -> III

L55 ANSWER 11 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 199543192 CHEMINFORMRX
TI Quinoxaline Chemistry. Part 4. 2-(R)-Anilinoquinoxalines as Nonclassical Antifolate Agents. Synthesis, Structure Elucidation and Evaluation of in vitro Anticancer Activity.
AU LORIGA, M.; FIORE, M.; SANNA, P.; PAGLIETTI, G.
CS Ist. Chim. Farm., Univ., I-07100 Sassari, Italy
SO Farmaco, 50(5), 289-301 (1995)
CODEN: FRMCE8 ISSN: 0014-827x
LA English

AB The title compounds, e.g. (VI), act as non-classical antifolic agents with modest to strong anticancer activity. The structure of intermediate (IIIa) is confirmed by an alternative synthesis.

RX(5) OF 12 ...H + K ==> L



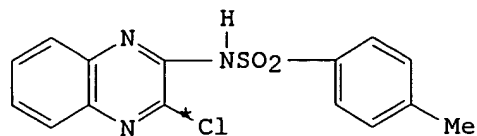
YIELD 69.0%

RX(5) RCT IV, **419652**
V, **14704** (24313-88-0)
SOL 182 (71-23-8), ProH
PRO VI, **419654**
YDS 69.0 %
T.KW REFLUX
KW arylation
NTE reaction:IV (V) -> VI, example: 1
CMT #E0100:(diastereom. mix.)

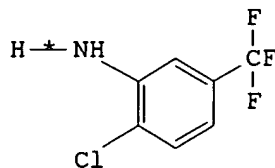
L55 ANSWER 12 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 199512215 CHEMINFORMRX
TI Synthesis, Structure and Chemical Properties of Some N-(3-Chloro-2-quinoxalyl)arylsulfonamides.
AU LITVINENKO, S. V.; SAVITCH, V. I.; BOBROVNIK, L. D.
CS Ukrainskii gos. univ. pishch. tekhnol., Kiev 252017, Ukraine
SO Khim. Geterotsikl. Soedin.(3), 387-392 (1994)
CODEN: KGSSAQ ISSN: 0453-8234
LA Russian
AB The title compounds, which exist as tautomeric mixtures of (III) and (IV), are converted into the derivatives (VI) and (VIII). Reaction of (III)/(IV) with arylamines of type (IX) and (XI) yields the tetracyclic products (X) and (XIII) via intramolecular cyclization.

10/088814

RX(11) OF 21 ...G + AB ==> AC...

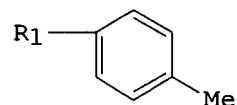
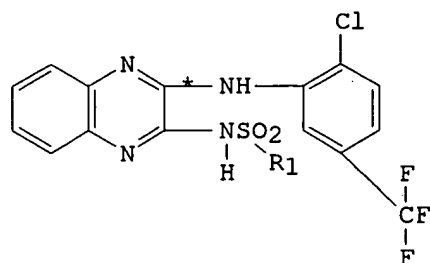


III



XI

(11) →



XII

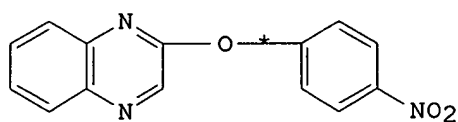
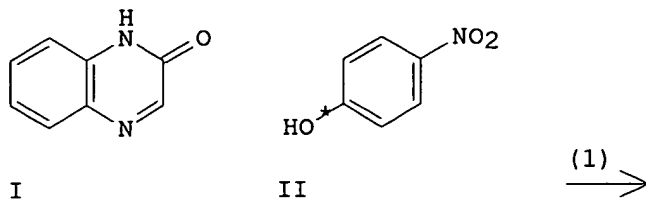
YIELD 83.0%

RX(11) RCT III, 371101
 XI, 18409 (121-50-6)
 SOL 76 (68-12-2), DMF
 PRO XII, 371111
 YDS 83.0 %
 T.KW REFLUX
 KW arylation
 NTE reaction:IIIb (XI) -> XII

L55 ANSWER 13 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
 AN 199429215 CHEMINFORMRX
 TI Synthesis of 2-(4-Nitrophenoxy)quinoxaline and Its Reactions with the Hydroxide Ion in Micellar Systems.
 AU CUENCA, A.; BRUNO, C.; TADDEI, A.
 CS Dep. Quim., Univ. Simon Bolivar, Caracas 1080-A, Venez.
 SO Tetrahedron, 50(7), 1927-1934 (1994)
 CODEN: TETRAB ISSN: 0040-4020
 LA English
 AB The title compound (III), which is generated from the quinoxalinol (I), reacts with OH⁻ in the presence and absence of micellar systems to afford the ketone (IV). Cationic micelles of cetyltrimethylammonium chloride and bromide and tetradecyltrimethylammonium chloride and bromide speed the reaction. In addition, it is found that the second-order rate constant in

water is higher than constants at the micellar pseudophase.

RX(1) OF 3 A + B ==> C...



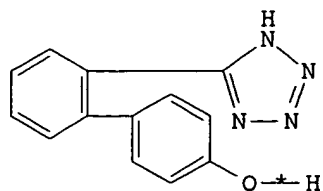
III

RX(1) RCT I, **323073**
 II, **3158** (100-02-7)
 STAGE(1)
 RGT 181 (10025-87-3), POCl₃
 461 (10026-13-8), PC15
 STAGE(2)
 RGT 1160 (1310-58-3), KOH
 YDS 57.0 %
 PRO III, **323074**
 KW arylation; O-arylation; etherification
 NTE reaction:I 2.(II) -> III
 CMT Ratio = 3.5:1 for products 1,2

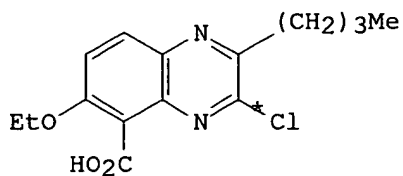
L55 ANSWER 14 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
 AN 199352202 CHEMINFORMRX
 TI Quinoxaline N-Oxide Containing Potent Angiotensin II Receptor Antagonists:
 Synthesis, Biological Properties, and Structure-Activity Relationships.
 AU KIM, K. S.; QIAN, L.; BIRD, J. E.; DICKINSON, K. E. J.; MORELAND, S.;
 SCHAEFFER, T. R.; WALDRON, T. L.; DELANEY, C. L.; WELLER, H. N.; MILLER,
 A. V.
 CS Bristol-Myers Squibb Pharm. Res. Inst., Princeton, NJ 08543-4000, USA
 SO J. Med. Chem., 36(16), 2335-2342 (1993)
 CODEN: JMCMAR ISSN: 0022-2623
 LA English
 AB A range of potent angiotensin II receptor antagonists containing a
 quinoxaline residue are prepared. Their efficacy is evaluated by
 radioligand binding studies using rat adrenal cortical membranes. It is
 found that analogs having a N-oxide function, e.g. (VI), are more potent
 antagonists than the parent nonoxidized compounds, e.g. (V).

RX(1) OF 3 A + B ==> C...

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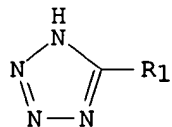
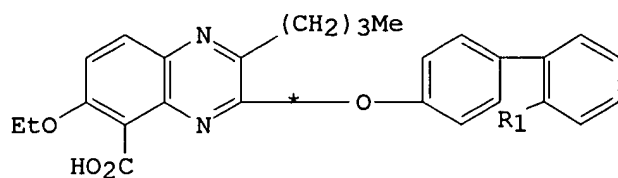


IV



II

(1) →



V

YIELD 84.0%

RX(1) RCT IV, **282214** (150368-30-2)
 II, **282213** (150368-44-8)
 RGT 1042 (534-17-8), Cs2CO3
 SOL 76 (68-12-2), DMF
 PRO V, **282215** (150368-48-2)
 YDS 84.0 %
 T 70.0 Cel
 TIM 15 hr
 KW arylation; O-arylation; etherification
 NTE reaction:IV (II) -> V

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